Validation documentation
BR IFAs e excipientes sólidos

HiperScan GmbH

March 7, 2025

Validation documentation of the chemometrics database of the near-infrared spectrometer *Apo-Ident*.
Report number: **175-2.9-2025-01**

Contents

Introduction **11**
Context of this document . . . 11
Criteria for the inclusion of substances . . . 12
Validation concept . . . 13
Model creation procedure and validation runs . . . 13
Particularities of individual substance classes . . . 16
Significance of testing with *Apo-Ident* . . . 16
Conclusion . . . 17

Explanation of terminology **18**

Summary **23**
Validation samples . . . 23
Validation results . . . 24

Validation reports **25**
4-hidroxibenzoato de metila . . . 25
4-hidroxibenzoato de propila . . . 33
Acetato de ciproterona . . . 39
Acetato de dexametasona . . . 47
Acetato de hidrocortisona . . . 55
Acetato de noretisterona . . . 81
Acetato de prednisolona . . . 89
Acetato de sódio tri-hidratado . . . 109
Acetato de zinco di-hidratado . . . 115
Acetilcisteína . . . 121
Aciclovir . . . 127
Ácido 4-aminobenzoico . . . 133
Ácido acetilsalicílico . . . 137
Ácido ascórbico . . . 145
Ácido aspártico . . . 153
Ácido benzoico . . . 157
Ácido bórico . . . 163
Ácido cítrico . . . 169
Ácido cítrico monoidratado . . . 193
Ácido esteárico 50 . . . 201
Ácido fólico hidratado . . . 207
Ácido fusídico . . . 213
Ácido glutâmico . . . 219
Ácido nicotínico . . . 225
Ácido oxálico . . . 231
Ácido salicílico . . . 237
Ácido sórbico . . . 261
Ácido tartárico . . . 269
Ácido tranexâmico . . . 279
Ácido ursodeoxicólico . . . 285
Alantoína . . . 291
Albendazol . . . 299
Álcoois de cera de lã . . . 305
Álcool cetoestearílico . . . 311
Álcool emulsificante não iônico . . . 327
Alfaestradiol . . . 333
Alopurinol . . . 345
Amido . . . 351
Amifampridina . . . 369
Amoxicilina tri-hidratada . . . 375

Anfotericina B . . . 381
Arginina . . . 387
Ascorbato de cálcio di-hidratado . . . 393
Ascorbato de sódio . . . 399
Aspartato de ornitina . . . 405
Aspartato monobásico de magnésio tetra-hidratado . . . 411
Azul patente V . . . 417
Bacitracina . . . 423
Baclofeno . . . 431
Barbital sódico . . . 437
Benzoato de estradiol . . . 441
Benzoato de sódio . . . 451
Benzocaína . . . 461
Besilato de anlodipino . . . 471
Betaína monoidratada . . . 475
Betametasona . . . 479
Bicarbonato de amônio . . . 485
Bifonazol . . . 491
Biotina . . . 497
Bitartarato de potássio . . . 503
Brometo de butilescopolamina . . . 509
Brometo de glicopirrônio . . . 515
Brometo de ipratrópio . . . 521
Brometo de neostigmina . . . 527
Bromidrato de dextrometorfano . . . 533
Bromidrato de hioscina . . . 539
Bromidrato de homatropina . . . 545
Budesonida . . . 549
Cafeína . . . 559
Canabidiol . . . 567
Cânfora racêmica/cânfora D . . . 583
Capsaicina . . . 591
Captopril . . . 597
Carbômero . . . 607
Carmelose sódica . . . 619
Celulose microcristalina . . . 627
Ceras/gorduras . . . 633
Cetoconazol . . . 669
Cianocobalamina/Metilcobalamina . . . 677
Ciclamato de sódio . . . 683
Ciclopirox olamina . . . 689
Ciclosporina . . . 697
Cistina . . . 705
Citrato de cafeína . . . 711
Citrato de cálcio tetra-hidratado . . . 717
Citrato de fentanila . . . 725
Citrato de magnésio . . . 731
Citrato de potássio . . . 737
Citrato de sildenafila . . . 747
Citrato de sódio . . . 757
Citrato monobásico de magnésio, hidratado . . . 775
Citrulina . . . 787
Clioquinol . . . 793
Cloranfenicol . . . 809
Cloreto de alumínio hexa-hidratado . . . 827
Cloreto de colina . . . 835
Cloreto de dequalínio . . . 839

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Cloreto de magnésio hexa-hidratado . . . 849
Cloreto de metacolina . . . 855
Cloridrato de ambroxol . . . 861
Cloridrato de amilorida di-hidratado . . . 873
Cloridrato de amitriptilina . . . 879
Cloridrato de arginina . . . 887
Cloridrato de benzidamina . . . 893
Cloridrato de bupivacaína . . . 901
Cloridrato de cetamina . . . 905
Cloridrato de ciprofloxacina . . . 911
Cloridrato de cipro-heptadina 1,5-hidrato . . . 917
Cloridrato de cisteína monoidratado . . . 921
Cloridrato de clindamicina . . . 927
Cloridrato de clonidina . . . 941
Cloridrato de cloreto de tiamina . . . 947
Cloridrato de clorprotixeno . . . 953
Cloridrato de clortetraciclina . . . 957
Cloridrato de cocaína . . . 965
Cloridrato de difenidramina . . . 971
Cloridrato de diltiazem . . . 977
Cloridrato de doxepina . . . 1001
Cloridrato de efedrina . . . 1007
Cloridrato de fenilefrina . . . 1013
Cloridrato de hidromorfona . . . 1019
Cloridrato de isoxsuprina . . . 1025
Cloridrato de lidocaína monoidratado . . . 1029
Cloridrato de lisina . . . 1049
Cloridrato de mepivacaína . . . 1055
Cloridrato de metadona . . . 1061
Cloridrato de metoclopramida monoidratado . . . 1075
Cloridrato de midazolam . . . 1081
Cloridrato de morfina . . . 1087
Cloridrato de nafazolina . . . 1095
Cloridrato de naloxona di-hidratado . . . 1103
Cloridrato de naltrexona . . . 1109
Cloridrato de noscapina monoidratado . . . 1113
Cloridrato de ornitina . . . 1117
Cloridrato de oxibuprocaína . . . 1123
Cloridrato de oxibutinina . . . 1129
Cloridrato de oxitetraciclina . . . 1137
Cloridrato de papaverina . . . 1147
Cloridrato de pilocarpina . . . 1153
Cloridrato de piridoxina . . . 1159
Cloridrato de prilocaína . . . 1165
Cloridrato de procaína . . . 1171
Cloridrato de propranolol . . . 1179
Cloridrato de quinina di-hidratado . . . 1191
Cloridrato de ropivacaína monoidratado . . . 1197
Cloridrato de sotalol . . . 1201
Cloridrato de tetracaína . . . 1205
Cloridrato de tetraciclina . . . 1221
Cloridrato de vancomicina . . . 1231
Cloridrato de xilometazolina . . . 1237
Cloridrato do ácido 5-aminolevulínico . . . 1245
Clorocresol . . . 1251
Clotrimazol . . . 1257
Colesterol . . . 1291

Concentrado seco de acetato de alfa-tocoferol 1299
Cromoglicato de sódio 1305
Curcumina 1311
Dexametasona 1315
Diacetato de clorexidina 1333
Diclofenaco sódico 1343
Dicloridrato de histamina 1353
Dicloridrato de octenidina 1359
Difenilciclopropenona 1373
Di-hidrocodeína[(R,R)-tartarato] 1379
Dihidrogenofosfato de potássio 1385
Dinitrato de isossorbida 40% 1389
Diosmina 1401
Dipropionato de beclometasona 1405
Dipropionato de betametasona 1411
Ditranol 1425
DL metionina 1435
Edetato de sódio 1439
Edetato dissódico de cálcio 1451
Eosina amarela 1457
Eritromicina 1463
Escina, hidrossolúvel 1497
Espironolactona 1503
Estearato de magnésio 1515
Estearato de zinco 1521
Estradiol hemi-hidratado 1525
Estriol 1535
Etinilestradiol 1545
Etossuximida 1551
Fampridina 1555
Fenazona 1561
Fenilbutazona 1567
Fenitoína 1573
Fenobarbital 1579
Finasterida 1585
Fluocinolona acetonida 1591
Fosfato de cálcio monobásico di-hidratado 1597
Fosfato de codeína hemi-hidratado 1603
Fosfato dibásico de clindamicina 2 1609
Fosfato dibásico de sódio di-hidratado 1615
Fosfato dissódico de prednisolona 1621
Fosfato sódico de riboflavina hidratado 1629
Frutose 1635
Fumarato de quetiapina 1649
Furoato de mometasona 1653
Furosemida 1673
Gabapentina 1679
Galactose 1683
Galato de bismuto, básico 1689
Gelatina, branca 1701
Glicerofosfato de cálcio 1707
Glicina 1715
Glicose 1721
Glicose monoidratada 1733
Gluconato de cálcio 1755
Gluconato de zinco 1763
Gluconato ferroso hidratado 1769

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Glutamina 1773
Glutationa 1779
Goma arábica, dispersão seca 1785
Gramicidina 1791
Griseofulvina 1797
Guaifenesina 1803
Hemifumarato de colina 1809
Hemissuccinato de doxilamina 1815
Hemissuccinato de prednisolona 1821
Hemitartarato de epinefrina 1827
Heparina sódica 1833
Hiclato de doxiciclina 1839
Hidrato de cloral 1845
Hidrocarbonato de potássio 1855
Hidroclorotiazida 1861
Hidrocortisona 1869
Hidroquinona 1893
Hidroxietilcelulose 1901
Hidroxitolueno butilado 1907
Histidina 1915
Ibuprofeno 1921
Indometacina 1927
Iodofórmio 1933
Iodopovidona 1943
Isoleucina 1951
Lactato de cálcio penta-hidratado 1957
Lactato de etacridina monoidratado 1963
Lactose monoidratada 1971
L-alanina 1989
Lecitina de soja (forma instantânea) 1993
Leucina 1999
Levedura de selênio 2005
Levocarnitina 2011
Levotiroxina sódica 2017
L-fenilalanina 2023
Lidocaína 2029
L-treonina 2045
Macrogol 1500 2051
Macrogol 4000 2057
Maleato de enalapril 2077
Maleato de feniramina 2083
Maltodextrina 2089
Manitol 2095
Melatonina 2121
Mentol 2135
Mesalazina 2153
Metamizol sódico monoidratado 2159
Metilcelulose 2165
Metilprednisolona 2177
Metionina 2183
Metoxisaleno 2189
Metronidazol 2199
Minoxidil 2227
Minoxidil sulfato 2249
Mio-inositol 2253
Monoestearatos 2257
Mupirocina cálcica 2267

Naproxeno 2273
Nicotinamida 2277
Nifedipina 2283
Nistatina 2287
Nitrato de miconazol 2303
Nitrato de nafazolina 2323
Nitrofurantoína 2329
Ofloxacino 2335
Omeprazol 2341
Orlistate 2349
Orotato de lítio monoidratado 2353
Orotato de magnésio di-hidratado 2359
Orotato de manganês di-hidratado 2365
Orotato de zinco di-hidratado 2371
Oxetacaína 2375
Palmitato de ascorbila 2381
Pancreatina, pulverizada 2391
Pantotenato de cálcio 2395
Paracetamol 2403
Pectina 2411
Piridoxal-5-fosfato 2415
Poloxâmero 2421
Povidona 2427
Prasterona 2435
Praziquantel 2443
Prednicarbato 2447
Prednisolona 2469
Prednisona 2489
Pregnenolona 2495
Prilocaína 2501
Progesterona 2505
Prolina 2525
Propifenazona 2531
Propionato de clobetasol 2537
Propionato de testosterona 2561
Proteinato de prata 2573
Quinolina amarela 2579
Resorcinol 2585
Riboflavina 2593
Sacarina sódica 2601
Sacarose 2609
Salicilato de sódio 2629
Serina 2635
Sorbato de potássio 2641
Sorbitol 2655
Sulfacetamida 2663
Sulfadiazina 2669
Sulfato de anfetamina 2675
Sulfato de atropina 2683
Sulfato de colistina 2689
Sulfato de condroitina sódico 2695
Sulfato de dexanfetamina 2699
Sulfato de gentamicina 2705
Sulfato de glicosamina cloreto de potássio 2723
Sulfato de magnésio hepta-hidratado 2727
Sulfato de manganês monoidratado 2733
Sulfato de neomicina 2737

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sulfato de polimixina B 2749
Sulfato de quinidina di-hidratado 2757
Sulfato de quinina 2763
Sulfato de salbutamol 2769
Sulfato de sódio deca-hidratado 2773
Sulfato de tobramicina 2779
Sulfato de zinco hepta-hidratado 2785
Sulfoguaiacolato de potássio 2791
Sulpirida 2797
Tacrolimo monoidratado 2801
Tanino 2807
Tartarato de L-Carnitina 2817
Tartarato de metoprolol 2821
Taurina 2827
Teofilina 2833
Teofilina etilenodiamina hidratada 2839
Testosterona 2845
Tetraborato de sódio 2853
Tetracaína 2859
Timerosal 2869
Timol 2875
Tirosina 2883
Tirotricina 2889
Tosilcloramida sódica 2895
Tretinoína 2901
Triancinolona 2917
Triancinolona acetonido 2923
Triclosan 2953
Triptofano 2983
Trometamol 2989
Tropicalamida 3001
Ubidecarenona 3007
Ureia 3013
Valerato de betametasona 3041
Valerato de estradiol 3071
Valina 3081
Vanilina 3087
Xilitol 3093
Xilose 3099

Appendix **3105**
Additional calibration samples (*Type A*) 3105
Additional validation samples (*Type B*) 3109
Additional validation samples (*Type C*) 3133
Requirements of validation 3261
Conformity of *Apo-Ident* with the *European pharmacopeia* 3262
Addition to the second-stage models 3263

References **3267**

Index **3269**

Introduction

The unequivocal proof of the identity of pharmaceutical raw materials based on a monograph or traditional alternative methods is work-intense, time-intense and economically often no longer makes sense. Near-infrared spectroscopy (NIR) provides a new means here. It enables relatively easy, fast and nonetheless safe identity testing via the preparation and evaluation of spectra.

The analysis system *Apo-Ident* was developed specially for pharmacy use. Pharmacists have the duty to check the identity of all raw materials for extemporaneous products in their pharmacies. This normally takes place based on the monographs for the respective substances in the European Pharmacopoeia. But also NIR spectroscopy is described in the European Pharmacopoeia as an identification method which, as opposed to the methods incorporated in the respective monographs, is approved for testing [1] (quotation translated)

> *with the prerequisite that the same results ("namely the determination of the identity" [2]),* (quotation translated) *are achieved as with the described methods and instruments.*

The *Apo-Ident* analysis system serves to identify raw materials for prescriptions in the defined manner according to *ApBetrO* [Pharmacies Rules and Regulations] §§ 6 and 11 at pharmacies (NIR spectroscopy as an alternative testing method). *Apo-Ident* consists of three components:

- An *NIR spectrometer*, which records the spectra of non-preprocessed raw materials in a measuring glass in diffuse reflection or transflection.
- The *QuickStep* spectroscopy software controls the instrument and records the spectra and user inputs via a pharmacy-specific software plug-in. It also generates the test protocol for documentation of the testing and storage of the printout to be signed in the pharmacy.
- The software module *IdentModule* incorporates *reference databases*. The spectra from the *QuickStep* software are presented to it for evaluation.

NIR spectroscopy is a very powerful analytical method. It is also able to establish the identity of several chemical compounds and mixes in as far as an appropriate database (technically correct: a chemometric model) was created. Identity testing with *Apo-Ident* is a very safe, very fast and easy to operate analytical method for testing a large number of raw materials.

Context of this document

The suitability of the instrument, method and database is proven as follows:

- *NIR spectroscopy as a method for identity testing:* The *Ph. Eur.* [3] describes NIR spectroscopy in *Section 2.2.40* as an analytical method which is also suitable for the identification of raw materials. Therefore, validation of the method as such is not necessary.
- *Performance of the instrument:* The *Ph. Eur.* [3] furthermore describes the apparatus and the testing of its performance in *Section 2.2.40*. The document *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4] compares the implementation by *Apo-Ident* with this monograph in order to prove that *Apo-Ident* meets the specifications of the Pharmacopoeia. Each individual instrument delivered to a pharmacy is qualified in accordance with the tests described in *"Control of Instrument Performance"*. In this test, the unit consisting of analysis instrument hardware and the *QuickStep* spectroscopy software is assessed. The result is documented in a test protocol which is kept at the pharmacy.
- *Validation of the database* is documented separately for each substance class. The report at hand documents the substance class *BR IFAs e excipientes sólidos*.

The *Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD)* [Working Group of German Pharmacy Inspectors] has clarified the following in its resolution dated October 16, 2013 ([5], quotation translated):

NIR is a testing method incorporated in the Pharmacopoeia. The testing quality depends on the quality of the database stored. The APD *views the use of NIR instruments in case of ensured validation of the databases used in conjunction with it as one of several options for identity testing.*

The *APD* defined more precisely ([6], quotation translated) on October 1, 2014:

The use of near-infrared is a recognised testing method according to Ph. Eur. 8. *For the use of NIR instruments in pharmacies for testing the identity of raw materials, sufficient and verifiable validation of the instrument used is required. The quality of the database stored by the instrument manufacturer is decisive for quality. Batch-specific differences with the same original substances must be taken into account if present.*

So NIR is basically suitable. The validity of the reference database is proven with the existing validation documentation.

Criteria for the inclusion of substances

This validation documentation describes the results of the validation of the reference database for the substance class *BR IFAs e excipientes sólidos*. Validation documentation is created for each published version of the reference database for all substance classes incorporated.

The reference database is incorporated in the software module *IdentModule*. During identification testing with *Apo-Ident*, spectra which are used for evaluation purposes are presented to it by the *QuickStep* software. In the same manner, the *IdentModule* is presented all validation spectra successively during the validation runs for evaluation purposes. The *IdentModule* responds respectively (without taking the initial assumption into account) with the identified substance or rejects it as unknown. The correctness of this response is checked for each possible initial assumption and counted.

The results are summarised for each substance and reproduced in this document. The core statement of this validation report is that the following criteria must be fulfilled for each database entry, so that *Apo-Ident* offers verification of identity by means of NIR for the relevant substance/substance group:

- The database is exclusively generated from spectra which have been recorded by *HiperScan GmbH* on traceable samples in pharmaceutical quality.
  - The samples are procured via typical pharmacy sources (*DAC III.2.: Bezugsquellennachweis für Rezepturbestandteile [reference source for prescription components]* [7]).
  - A valid manufacturer's certificate exists (content, purity and identity of the batch).
  - The identity was confirmed by a certified test laboratory or *HiperScan GmbH*.
- Each version of the reference database (every update) is validated in-full.
  - Calibration spectra (*Type A*), other spectra recorded under the control of *HiperScan GmbH* (*Type B*), and spectra from the field (*Type C*) are presented to the *IdentModule* for evaluation in three separately evaluated validation runs.
  - Here, no single *false positive* result may arise.
  - Here, the various substance classes are also tested for reciprocal rejection, where this is objectively justified (see *Summary* section).
- In the validation with spectra recorded under the control of *HiperScan GmbH*, spectra of at least one independent sample must be considered, i.e. spectra from a batch whose spectra have not been used for the generation of the database. In addition, the set of *Type A* and *Type B* spectra must originate from at least three different batches.
- Spectra of additional substances may be used for the generation of the database even though they will not be offered for identification by this database. The purpose is the reliable distinction from these substances.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- Any positive result of *Apo-Ident* confirms the identity of the substance/substance group and distinguishes it from all other substances of the database. In the case of substance groups, the result is ambiguous: Distinction from all substances not belonging to the group is proven. The substance is identified as a member of this group. However, within the substance group, it is not possible to reliably classify which substance has been tested.

- The criteria for clear identifiability are a specificity of 100 % (true negative rate) and a minimum distance in the distance matrix. See 2. d) under Model creation procedure and validation runs.

Validation concept

Chemometrics is a statistical technique for the extraction of relevant chemical information from spectra. In mathematics, this method is described as *multivariate data analysis*. Chemometrics proceeds here as follows:

1. Collection of spectra for the *calibration sample*. The results (identities) of the calibration sample must be known. The calibration samples must be representative for the samples which are to be evaluated later. Therefore, they must take the various possible (physical) compositions into account. (Therefore, sourcing calibration samples for NIR from the specialist trade is superior to the use of CRS reference substances.)

2. The first mathematical step is *calibration*. Here, the chemometric model is calculated from the *calibration sample spectra* (reference spectra) and limits as well as some parameters are stipulated. The chemometric model is used later to calculate the analysis result (*prediction*).

3. Collection of further spectra for the *validation sample* which should be independent of the *calibration sample*. The results (identities) of the *validation sample* must also be known. The textbook suggests a random sample with a normal scope of 25 % to 50 % of the *calibration sample* [8].

4. The second technical data step is *validation*. Here, the chemometric model created is evaluated based on the spectra of the *validation samples*. As validation parameters for the identification, the *Ph. Eur. Section 2.2.40* [3] specifies the specificity and robustness.

The validation step according to the textbook has the target of estimating the performance capability of the model created based on a random sample. In order to achieve the best possible precision, attention is paid to the calibration sample. In the field of pharmaceuticals, the safety of the method has priority. In order to be able to *validate* the model within the regulatory scope, the validation step must include probative force. For this purpose, the validation sample must be *representative and complete* in order to enable the testing of all cases.

A *sufficient number of batches* must be secured for validation because validation finally proves whether the number of batches in calibration suffices.

Each substance is validated individually. The validation results are documented per substance in this document. Moreover, the documents show how many and which batches have been used for creating the model or model validation.

At least one certificate is taken in for each substance from an accredited test laboratory for the independent testing of identity of the sample. The identification number of the corresponding test certificate is listed in the report, enabling traceability of a substance tested according to the monographs in the Pharmacopoeia.

Model creation procedure and validation runs

The safety of the chemometric models is guaranteed by several measures during model creation, of which the validation step is the final one. Normally, the procedure is as follows. It is in particular valid for the active pharmaceutical ingredients (APIs) *solid API excipients*, *liquid/semi-solid API excipients (with a test certificate)* and *narcotics - solid medicinal substances*. If, for individual substance classes, variations are required, they are depicted in the section *Particularities of individual substance classes*.

1. Collecting the reference spectra (calibration sample)

a) Procurement of the samples from the same sources from which pharmacies source their raw material for compounding (Caelo, Fagron, Euro-OTC, ..., see also *DAC III.2. Bezugsquellennachweis für Rezepturbestandteile* [Sources of supply for compounding] [7]).

b) Testing the suitability according to *ApBetrO* [Pharmacies Rules and Regulations] §§ 6, 11, that is to say the availability of a valid manufacturer certificates via identity, purity and contents of the batch.

c) Recording standard 40 spectra of the sample in different positions, as a standard on four instruments. Here, handling and presentation of the samples as later in the pharmacy.

d) Visual checking for anomalies in the spectra. In case of indications of measurement errors, measurement must be repeated. If a signature is missing in the spectrum, the substance may be excluded from the start as not promising (the spectra are nonetheless entered in the database validation as independent *Type B* spectra).

e) Testing identity. For each substance, a certificate of correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the respective following substance page of this validation documentation the *Mahalanobis distance* to this reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance. Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

   HiperScan GmbH cooperates with some suppliers as follows: the raw materials supplier takes a sufficiently large sample in his incoming goods area so that part of it can be used for recording the NIR spectra. The remainder of the sample goes to analytics for market approval. The manufacturer's batch certificate emerges from these identity, contents and purity tests, which consequently also prove the correct identity of the NIR reference sample. Therefore, the NIR spectra are suitable for structuring the database *(Type A)* and can also optionally be used for validation *(Type B)*. The samples which this applies to are marked in the validation report with a footnote.

f) If the identity of the new sample is proven, it is declared as a reference sample and the spectra are approved for structuring the database.

2. Generating the chemometric models (calibration)

a) Determination of the transformation matrix from the reference spectra using variance maximisation [8, 9]. (*All* reference spectra are always included, even if only a few spectra are added for an update.) All reference spectra receive the same data pre-treatment, which is also later applied to all measurement spectra in the field (in the pharmacies).

b) Checking that the number of principal components used is still sufficient.

c) Calculating the limits for each substance from the spread of the reference spectra. The calculation regulation is identical for each substance in a substance class.

d) Checking the distances between the limits of the separable substances: The distance matrix contains the *Mahalanobis distances* from each substance to each other. The values in a bidirectional manner are different in each case because the spread of the initial substance is included. If a distance is smaller than the minimal distance, the substances are not considered to be reliably separable. The minimal distance is set at 9. The developer of the model may specify a larger minimal distance (one value for the entire *chemometric model*), to increase the selectivity.

e) Verification of the model using the reference spectra. No *false-positive* results are permitted.

f) If one of the criteria is violated (d) *Minimum distance between two substances undershot* or (e) *One substance is identified as another*, the database developers decide which of the following options to apply:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- They remove both substances from the database. (The spectra remain in the validation and may also be included when generating the model. However, they are not offered for testing.)
- They form a substance group of several substances which cannot be reliably separated. The result is then ambiguous: The chemometric model determines that the sample is one of the substances in the group and not another substance. However, it cannot determine which of the group members it is. In order to determine the clear identity, the user must carry out a suitable additional analysis.
- They create another *chemometric model* with a smaller scope, in which at least all substances of the non-separable substance group are included (second-stage model). Second-stage models are only called up if the first stage has established that only one of the substances included in the second-stage model can be involved. The second-stage models are documented in the appendix *Addition to the second-stage models*.

g) If *chemometric models* that fulfil both criteria (distance matrix and no *false positives*), are available for all substance classes, they are combined with the evaluation algorithms to form an *IdentModule* and encoded. This unit can no longer be changed. Its overall function is checked by the validation.

3. Set of validation spectra (validation samples)

The following is provided for validation:

a) *Type A*: The reference spectra = calibration spectra from which the database was generated. These also include spectra from substances which the *chemometric model* should not identify, but were also recorded during generation in order to increase selectivity. (As a result, the model "learns" to differentiate from other substances which are actually unknown to it.)

b) *Type B*: Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database. These also include reference spectra of other substance classes, and spectra that are not used as reference spectra. Samples are considered to be independent, if they originate from a batch, of which no spectra have been used for the generation of the database. (Up to *IdentModule 2018-01*, samples were still considered independent if the sampling was done independently, i.e. if they originate from another sales container.)

c) *Type C*: Spectra from the field, which have not been recorded under the control of *HiperScan GmbH* and have not been used for the generation of the database. The spectra include not only substances of the substance class to be tested, but also substances from other classes.

All manufacturers' batches from which spectra are used for the validation are listed by substance in this document: for substances included in the substance class *BR IFAs e excipientes sólidos* in the respective validation reports; otherwise in attachments *A*, *B* and *C*.

Furthermore remains valid: validation spectra may only be removed if an error in the spectrum can be proven. Here, the spectra are not deleted, but instead placed on a *blacklist* incorporating the reason, date and initials in the commentary.

The section *Particularities of individual substance classes* treats the other substance classes from which *Type B* and *Type C* spectra are cited for validation purposes.

4. Validation runs and approval

a) Validation spectra are transferred holistically to the *IdentModule* for evaluation in the same way as the spectroscopy software *QuickStep* transfers measured spectra.

b) Following the provision of each spectrum, the *IdentModule* responds as to whether it has recognised a substance and which substance was recognised.

c) The correctness of this response is checked for each possible initial assumption (each measurable substance with the substance class) and counted according to *true negative*, *false negative*, *true positive* and *false positive*. These figures are provided for each substance and additionally in the section *Summary*, separated according to types *A*, *B* and *C* .

d) No *false positive* results whatsoever are permissible.

e) If the criterion is also met for all substance classes, the *IdentModule* is approved.

Particularities of individual substance classes

Basically, *HiperScan GmbH* procures and tests the manufacturer's certificate for the batch, commissions external testing of the identity of the sample or carries it out independently and stores the certificates. As described, this process is established for the Pharmacopoeia substances, that is to say for substance classes **APIs & excipients, solid**, **APIs & excipients, liquid/semi-solid (with analysis certificate)** and **Narcotic substances, liquid/semi-solid**. Therefore, *HiperScan GmbH* is able to furnish proof of the identity of the reference samples. In case of manufacturer-specific substance classes and others, individual steps are organised differently in-part:

The substance class **APIs & excipients, liquid/semi-solid (other)** (often described as cosmetics) incorporates substances for which no specification of the requirements of the pharmaceutical quality is determined, neither in a Pharmacopoeia monograph, a DAC/NRF monograph nor via a manufacturer's specification. Consequently, neither the identity nor contents can be tested independently. No certificates whatsoever exist for the reference samples. So here, merely the matching of the sample with former samples of this product is established and confusion with the other substances is ruled-out. (If the manufacturer of such a substance prepares a specification, determines testing methods and provides manufacturer's certificates in accordance with *ApBetrO* [Pharmacies Rules and Regulations] §§ 6, 11, *HiperScan GmbH* can assign the substance to the substance class *APIs & excipients, liquid/semi-solid (with analysis certificate)* again in the future).

Substance class **HCK – nutritional supplements (Hepart)** contains the HCK micro-nutrients from the Swiss company *Hepart AG*. *HiperScan GmbH* receives the reference samples directly from the manufacturer. For each reference sample, *HiperScan GmbH* also receives manufacturer's certificates and keeps these. New checking of the identity of the reference sample is not carried out by *HiperScan GmbH*. The identity of the reference samples is therefore documented by *Hepart AG*. The spectra of all batches provided by *Hepart AG* are recorded by *HiperScan GmbH* and entered in the database.

All the manufacturer's batches are used for the generation and validation of the substance class *HCK*. The expected variation is also represented in the generation and validation if there are less than three batches.

Significance of testing with *Apo-Ident*

The analysis result is determined using sophisticated statistical methods according to state-of-the-art science and technology. Chemical and pharmaceutical knowledge is applied for the selection of the samples from which the calibration spectra and validation spectra are recorded. Otherwise it does not influence the further steps of model creation.

Verbally, the statement of the analysis result can be expressed as follows. Here *"the spectra match"* means that the criteria *Mahalanobis distance*, *outlier analysis* and *correlation* are met as shown in *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]. "The spectra do not match", on the other hand, means that at least the criterion *Mahalanobis distance* is not met.

The positive analysis result *"was identified as ..."* is very meaningful because both the quantity of substances to be taken into account and the number of underlying samples is very comprehensive.

1. The spectrum of the sample measured matches spectra of the defined substance.

2. The spectrum of the sample measured does not match any spectrum of any other substance in this substance class. Therefore, all other substances can be clearly ruled-out.

3. As the spectra from other substance classes were used for validation, it is proven that no spectrum of one of these other substances matches the defined substance. (All substance classes with which a spectrum comparison is possible and makes sense are used for validation. This is documented for each substance class in the section *Summary*.)

4. If the defined substance belongs to a *substance group* which in itself is not clearly separable with *Apo-Ident*, matching with the spectra of one or several substances in this group is confirmed.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Which of these substances it actually is cannot be determined clearly. All other substances are excluded analogous to 2 and 3.

On the other hand, a negative analysis result *"was not identified as ..."* means:

1. The substance offered could not be recognised based on the spectrum of this sample.
2. The identity of this sample is not confirmed.
3. Testing must be repeated in accordance with the specifications of the Pharmacopoeia.

Conclusion

NIR spectroscopy is a testing method incorporated in the Pharmacopoeia. In case of successful database validation, it is a possible method for identity testing [5]. *Apo-Ident* meets the criteria of the *European Pharmacopeia* as a near-infrared spectrometer and proves the validity of the reference database with the existing validation documentation. This means that *Apo-Ident* can be used as an alternative testing method for testing raw materials at pharmacies.

Explanation of terminology

The following section serves to explain or define specialist terminology which is required in order to understand this document. If necessary, definitions for the analysis system *Apo-Ident* are defined more precisely.

The term database is used in this document exactly as in the *Ph. Eur. Section 2.2.40* [3] synonymous with chemometric model. In order to differentiate the databases which are relatively independent of each other, *HiperScan GmbH* frequently also uses the term substance class (primarily in the plural). On the other hand, the spectra used to structure the database are termed spectrum collection and not database.

Substance classes are units of the organisational structure of the *IdentModule*. The substance classes are substance databases which are also broadly independently subscribable. On the one hand, the liquid and semi-solid substances are separated from the solid powders because they are measured against different references and therefore the spectra cannot be compared. On the other hand, for example the Pharmacopoeia substances are kept separated from the manufacturer-specific database HCK micro-nutrients from the Swiss company *Hepart AG*.

The individual substance classes need only be limited against each other in-part. Often, no risk of confusion exists because they can only be procured from different sources. On the other hand, in several cases we handle substances which need not be distinguished. For example, *Angelica root oil* of the substance class *APIs & excipients, liquid/semi-solid (with analysis certificate* neither needs to be delimited from *Angelica root oil* of the substance class *APIs & excipients, liquid/semi-solid (other)* nor is matching required. Respectively one single chemometric model is behind a substance class. (Even if several reciprocally secured chemometric models would be permissible.) The terms *substance class*, *chemometric model* and *databases* are mostly used here as synonyms.

A substance group respectively summarises all the substances within a substance class which cannot safely be distinguished from one another based on their NIR spectra. However, all the other substances in the database can be excluded.

The formation of subgroups is mentioned in the *Ph. Eur. Section 2.2.40* [3]. In this manner, technical restrictions in case of extensive databases can be avoided and it is possible to prepare individual subgroups with different spectrum pre-treatment. Validation of the subgroups against each other is required. *HiperScan GmbH* has solved these technical restrictions and doesn't use any subgroups within a substance class any longer.

Principal component analysis (PCA) [8, 9] is a multivariate statistics process or multivariate data analysis. It serves to structure, simplify and illustrate comprehensive data records by describing a large number of statistical variables by describing a lower number of linear combinations (the *principal components*) which are as significant as possible. In the *Apo-Ident IdentModule*, *PCA* is used to evaluate the recorded spectrum data (corresponding with *Ph. Eur. 2.2.40* [3]).

The term validation is defined in both relevant contexts here with different (even if related) meanings.

Within the sense of the expert discipline of *chemometrics*, validation is a process step when creating a chemometric model: after a transformation matrix, limits and various parameters have been calculated or determined from a set of reference spectra during the course of the calibration step [8, 9], the validation step determines the performance capability of the model (selectivity, precision, ...) based on the validation spectra. Normally, random sampling is planned here. In order for the validation to gain strength of proof, the validation spectrum set must be selected with an appropriately wide scope (*representative* and *complete*). The terms *validation run* and *validation step* always actually mean the process step in this sense.

In the regulatory sense (of pharmaceutical production), validation is the documented proof that a process or system meets the previously specified requirements reproducibly when applied practi-

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

cally. In this sense, the *Apo-Ident* databases only become validated databases with the validation documentation, which this document is part of.

The *European Pharmacopeia* uses the term validation in *Section 2.2.40* within the sense of the specialist discipline of *chemometrics* [3].

The robustness of a process is the property of only being influenced by environmental fluctuations (e.g. temperature or humidity) a little. A method is robust if the environmental conditions do not or hardly falsify the final result.

The specificity of a classification (of a chemometric model) is the true negative rate.

The recognition rate (also sensitivity) is the true positive rate. It defines in how many percent of cases a correctly set up substance is actually confirmed.

The true negative rate describes the share of spectra correctly classified as non-identity during validation. This is equivalent to correct classification. It means that a substance A within identity checking as substance B is judged as *"not identified"*. The *true negative rate* is equivalent to the conditional frequency

$$h(\text{rejected}|\text{genuinely no identity}) = \frac{r_n}{r_n + f_p}$$

with r_n as the total number of *true negative* classifications and f_p as the total number of *false positive* classifications. For successful validation of an *IdentModule*, all spectra presented belonging to this category must be classified as *not in accordance*.

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of this number. The weight of each spectrum of a substance/substance group i therefore results as

$$w_i = \frac{1}{n_i}$$

with n_i number of spectra in this substance/substance group. This weighting ensures that the overall result cannot be enhanced by adding especially large numbers of spectra from easily separable substances.

The true positive rate describes the share of spectra correctly classified as identity during validation. This is equivalent to correct classification. It means that a substance A within identity checking as substance A is judged as *"identified"*. The *true positive rate* is equivalent to the conditional frequency

$$h(\text{identified}|\text{genuine identity}) = \frac{r_p}{r_p + f_n}$$

with r_p as the total number of *true positive* classifications and f_n as the total number of *false negative* classifications. The *true positive* rate is a measure for the recognition rate of the validated *Apo-Ident IdentModule*.
In order to ensure that each substance is received with the same weight, the spectra are weighted as described for the true negative rate.

The true negative result describes a spectrum correctly classified as non-identity during validation. It is equivalent to correct classification. It means that a substance A within identity checking as substance B is judged as *"not identified"*.

The false positive result describes a spectrum falsely classified as non-identity during validation. This is the most critical type of possible false classification. It means that a substance A within identity checking as substance B is judged as *"identified"*. For successful validation of an *IdentModule*, a number of false positive events of zero are demanded for all spectra entering the validation.

The true positive result describes a spectrum correctly classified as identity during validation. It is equivalent to correct classification. It means that a substance A within identity checking as substance A is judged as *"identified"*.

The false negative result describes a spectrum falsely classified as non-identity during validation. It is equivalent to false classification. It means that a substance A within identity checking as substance A is judged as *"not identified"*.

The 'Rule of Three' says that with a probability of 95 % the next random sample of the same size no more than three false results are to be expected if no false result existed in the existing random sample [10, 11].

The *specificity* and *recognition rate* are determined both globally and from the validation runs for all substances. The information is supplemented with the hypothetical value if there had been three false results more. The percent information is provided in parentheses with the "greater than" symbol '>', e.g. *specificity* 100.000 % (>99.983 %) if 17 567 false spectra have been presented without one single *false positive* result. The larger the statistical basis, the lower the influence of the hypothetical false results.

The Mahalanobis distance is a distance measure between two points in n-dimensional vector space. Here, the respective direction component of the distance to *standard deviation* [12] of an n-dimensional distribution is standardised. In case of the *principal component analysis* [8, 9] this standardisation relates to the distribution of the respective calibration data set for a classification (substance/substance group) in the *principal component space* [8]. The *Mahalanobis distance* of a point (mapping of a spectrum) $\vec{y}$ in the n-dimensional principal component space to the expected value of an n-dimensional distribution $\mathbf{X}$ then results as

$$d(\mathbf{X}, \vec{y}) = \sqrt{(\bar{\mathbf{X}} - \vec{y})^T \mathbf{S}^{-1} (\bar{\mathbf{X}} - \vec{y})} \qquad \text{with} \qquad \mathbf{X} \in \mathbb{R}^{m \times n}, \vec{y} \in \mathbb{R}^m$$

[13]. Here, m is equivalent to the number of principal components used (dimension of the principal component space) and n the number of measurements existing in the calibration data set (spectra). $\bar{\mathbf{X}}$ is the expected value of the resulting distribution for the calibration data set (the average value of n measurements received). $\mathbf{S}^{-1}$ is the inverse covariance matrix [12] for distribution $\mathbf{X}$.

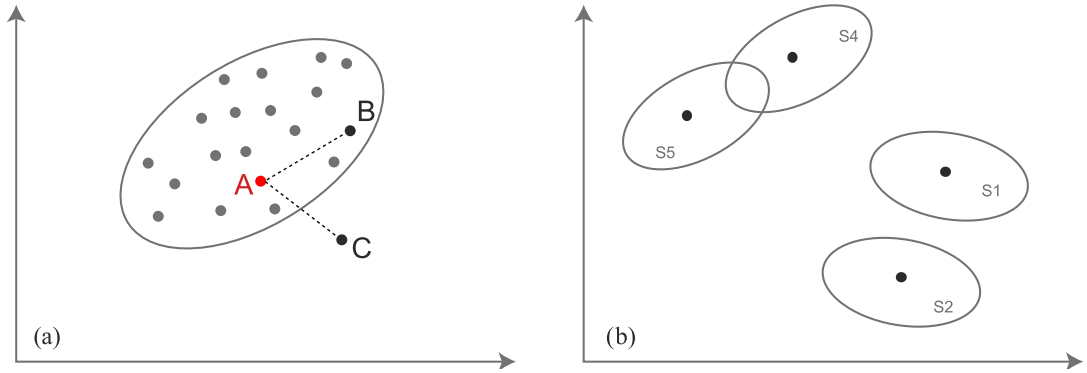


Figure 1: (a) The *Mahalanobis distance* from A to B is less than from A to C. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

The *Mahalanobis distance* offers advantages compared to the *Euclidean distance*: For the calculation of the distance it takes the statistical properties of a data point distribution (measurement series), i.e. average value, variance and covariance of the data points [14] into account. The *Mahalanobis distance* is applied while creating the reference database for evaluating the spectra from different samples of a substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

A chemometric model is a classifier based on statistical methods [8, 9]. Through the respective algorithm used (e.g. *Principal Component Analysis*, *Cluster Analysis*), a maximum of chemical information is extracted from measurement data. Here, systematical or physical disturbances are eliminated using appropriate data pre-processing [15, 16].

At several places in this document, in order to simplify understanding, the term database is used instead of *chemometric model* – in the same manner as in the *Ph. Eur. Section 2.2.40* [3].

A sample (with its own sample ID) refers to substance in a sales container. Repeated sampling from the same sales container is listed under the same sample ID. (The suffix "SI" is not part of the sample ID.) Several samples may originate from the same batch. Samples are called "independent", if they originate from a batch, of which no spectra have been used for the generation of the database. (Up to *IdentModule 2018-01*, samples from different sales packages were considered to be independent.) The information above the list of validation spectra now includes also the number of batches that deliver independent samples for the validation (for both *Type B* and *Type C*).

In case a supplier takes a sample for testing from its incoming goods and splits it to multiple laboratory containers, the substance in all laboratory containers will still be ascribed to the same sample. *HiperScan GmbH* only uses one of the subsamples.

Reference samples are used to structure the database. The *reference spectra* originate from these samples. In chemometric technical jargon you would normally say: For *calibration*, a *chemometric model* is generated from the *calibration spectra* recorded from the *calibration samples*, whose quality is subsequently assessed in validation.

Reference samples are procured via typical pharmacy sources. Their identity is tested. The *reference spectra* are recorded by *HiperScan GmbH*. The documentation also includes the manufacturer's name and batch number.

Reference samples are clearly identified by a sample ID. Samples without sample ID may not be used as *reference samples*.

Summary

A total of 593 865 spectra from 54 984 different batches for a total of 953 substances were used to validate the substance class *BR IFAs e excipientes sólidos*.

Validation samples

The validation samples can be categorised as follows:

Type A Calibration spectra. These are the spectra used to generate the chemometric model. They were recorded by *HiperScan GmbH*. Detailed information regarding the batches or samples can be found in the following validation reports under *calibration samples* and under *Type A*. Further information is listed in *Appendix A*.

Substance class	Substances	Batches	Spectra
IFAs e excipientes sólidos	394	2663	142 702
IFAs e excipientes sólidos (BR)	10	15	640
Substâncias sólidas sujeitas a controle especial	13	66	6000
Classificador específico 26188	17	37	1750
Fármacos	52	61	2660

From category *A* a total of 153 752 spectra from 2842 batches for a total of 486 substances were taken into account for validation.

Type B Spectra from independent samples which are not included in database generation. These spectra were recorded by *HiperScan GmbH*. Detailed information regarding the batches or samples can be found in the following validation reports in the section *Type B* or in *Appendix B*.

Substance class	Substances	Batches	Spectra
IFAs e excipientes sólidos	530	3333	168 452
IFAs e excipientes sólidos (BR)	27	46	2220
Substâncias sólidas sujeitas a controle especial	17	66	5040
Classificador específico 26188	12	23	1019
Fármacos	250	575	25 703
Chemikalien fest	8	8	320

From category *B* a total of 202 754 spectra from 4051 batches for a total of 844 substances were taken into account for validation.

Type C Spectra from independent samples which are not included in database generation. *Apo-Ident* customers carried out the measurements. Detailed information regarding the batches or samples can be found in the following validation reports in the section *Type C* or in *Appendix C*.

Substance class	Substances	Batches	Spectra
IFAs e excipientes sólidos	418	43 125	220 517
Substâncias sólidas sujeitas a controle especial	15	894	2428
Fármacos	286	6038	14 406
Classificador específico 26188	3	7	8

From category *C* a total of 237 359 spectra from 50 064 batches for a total of 722 substances were taken into account for validation.

Validation results

The validation runs checked whether all substances/substance groups in the substance class *BR IFAs e excipientes sólidos* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, the matching of all relevant spectra of various substances with the substances/substance groups in the substance class *BR IFAs e excipientes sólidos* was checked and the correctness of the results was evaluated. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	146 949	53	55 531 166
Type B	0	155 623	220	73 402 459
Type C	0	216 666	2771	85 708 168

All substances/substance groups in the substance class *BR IFAs e excipientes sólidos* can be clearly distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.000 00 % (> 99.999 97 %)	99.977 34 % (> 99.974 49 %)
Type B	100.000 00 % (> 99.999 98 %)	99.696 72 % (> 99.692 34 %)
Type C	100.000 00 % (> 99.999 73 %)	98.402 96 % (> 98.343 35 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**4-hidroxibenzoato de metila**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20345-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

4-hidroxibenzoato de metila; Methylis parahydroxybenzoas

Special notes

When selecting the *4-hidroxibenzoato de metila* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
4-hidroxibenzoato de metila	6	18	139

Second-stage model

For differentiation of the substance/substance group *4-hidroxibenzoato de metila* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *4-hidroxibenzoato de metila* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	104,35	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *4-hidroxibenzoato de metila* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *4-hidroxibenzoato de metila*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	4-hidroxibenzoato de metila	11090034	20693	40	20110428
Caelo	4-hidroxibenzoato de metila	181769	24223	40	20180824*
Euro OTC	4-hidroxibenzoato de metila	1205025-01	20697	40	20120601
Euro OTC	4-hidroxibenzoato de metila	1601037	22305	60	20160119*
Fagron	4-hidroxibenzoato de metila	14L30-T01-018345	23223	40	20150309
Fagron	4-hidroxibenzoato de metila	19B05-T03-062158	24588	40	20190228

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *4-hidroxibenzoato de*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

metila. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 790 spectra of 21 reference samples from the substance/substance group *4-hidroxibenzoato de metila*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	4-hidroxibenzoato de metila	13268813	21439	60
Caelo	4-hidroxibenzoato de metila	15063820	23216	40
Caelo	4-hidroxibenzoato de metila	171581	23317	40
Caelo	4-hidroxibenzoato de metila	191302	24711	40
Caelo	4-hidroxibenzoato de metila	192334	24886	40
Caelo	4-hidroxibenzoato de metila	22000388	26117	40
Caelo	4-hidroxibenzoato de metila	22003498	26475	40
Caelo	4-hidroxibenzoato de metila	23000896	26852	40
Caelo	4-hidroxibenzoato de metila	23003474	27102	40
Euro OTC	4-hidroxibenzoato de metila	1706005	23703	40
Euro OTC	4-hidroxibenzoato de metila	1807009	24148	40
Euro OTC	4-hidroxibenzoato de metila	1902025	24568	40
Euro OTC	4-hidroxibenzoato de metila	1909009	24852	40
Euro OTC	4-hidroxibenzoato de metila	2004013	25155	40
Euro OTC	4-hidroxibenzoato de metila	2010001	25409	40
Euro OTC	4-hidroxibenzoato de metila	2304023	26639	40
Fagron	4-hidroxibenzoato de metila	22L02-B13-226168	26548	40
Gatt-Koller	4-hidroxibenzoato de metila	23J00964	27100	30
Caelo	4-hidroxibenzoato de metila	22000388	26117SI	20
Caelo	4-hidroxibenzoato de metila	22003498	26475SI	20
Fagron	4-hidroxibenzoato de metila	22L02-B13-226168	26548SI	20

- 201 294 spectra from a total of 4027 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 694 spectra from 475 *Apo-Ident* customers from 141 batches from the substance/substance group *4-hidroxibenzoato de metila*.
- Among them are spectra of independent samples from 136 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	4-hidroxibenzoato de metila	2010001-02	4
	4-hidroxibenzoato de metila	22000388006	1
	4-hidroxibenzoato de metila	22000388010	1
	4-hidroxibenzoato de metila	22003498003	11
	4-hidroxibenzoato de metila	22J02568	1
	4-hidroxibenzoato de metila	23000896007	1
AHD	4-hidroxibenzoato de metila	12251624	1
AHD	4-hidroxibenzoato de metila	17158101	1
AHD	4-hidroxibenzoato de metila	17343002	1
AHD	4-hidroxibenzoato de metila	22003498003	1
AHD	4-hidroxibenzoato de metila	2300896007	1
Anzag	4-hidroxibenzoato de metila	11345115	1
apo-ident	4-hidroxibenzoato de metila	1706005-01	1
Bombastus	4-hidroxibenzoato de metila	1212011-01	1
Caelo	4-hidroxibenzoato de metila		2
Caelo	4-hidroxibenzoato de metila	1000076005	1
Caelo	4-hidroxibenzoato de metila	1108211930	1
Caelo	4-hidroxibenzoato de metila	11090003	1
Caelo	4-hidroxibenzoato de metila	11090030	1
Caelo	4-hidroxibenzoato de metila	11090031	4
Caelo	4-hidroxibenzoato de metila	111003301	1
Caelo	4-hidroxibenzoato de metila	11345103	1
Caelo	4-hidroxibenzoato de metila	11345115	7
Caelo	4-hidroxibenzoato de metila	11345120	2
Caelo	4-hidroxibenzoato de metila	12081502	1
Caelo	4-hidroxibenzoato de metila	12251605	2
Caelo	4-hidroxibenzoato de metila	12251611	1
Caelo	4-hidroxibenzoato de metila	12251619	1
Caelo	4-hidroxibenzoato de metila	12251624	5
Caelo	4-hidroxibenzoato de metila	1251624	1
Caelo	4-hidroxibenzoato de metila	13081308	1
Caelo	4-hidroxibenzoato de metila	13268802	1
Caelo	4-hidroxibenzoato de metila	13268803	1
Caelo	4-hidroxibenzoato de metila	13268804	9
Caelo	4-hidroxibenzoato de metila	13268809	5
Caelo	4-hidroxibenzoato de metila	13268813	7
Caelo	4-hidroxibenzoato de metila	13268815	1
Caelo	4-hidroxibenzoato de metila	13268819	1
Caelo	4-hidroxibenzoato de metila	13268821	1
Caelo	4-hidroxibenzoato de metila	14120207	1
Caelo	4-hidroxibenzoato de metila	14120208	5
Caelo	4-hidroxibenzoato de metila	15063802	8
Caelo	4-hidroxibenzoato de metila	15063803	1
Caelo	4-hidroxibenzoato de metila	15063806	8
Caelo	4-hidroxibenzoato de metila	15063812	3
Caelo	4-hidroxibenzoato de metila	15063813	2
Caelo	4-hidroxibenzoato de metila	15063818	4
Caelo	4-hidroxibenzoato de metila	15063819	4
Caelo	4-hidroxibenzoato de metila	15063819/1210217	1
Caelo	4-hidroxibenzoato de metila	15063820	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	4-hidroxibenzoato de metila	15222203	5
Caelo	4-hidroxibenzoato de metila	15298101	1
Caelo	4-hidroxibenzoato de metila	15298102	12
Caelo	4-hidroxibenzoato de metila	15444905	1
Caelo	4-hidroxibenzoato de metila	15444911	1
Caelo	4-hidroxibenzoato de metila	15444913	4
Caelo	4-hidroxibenzoato de metila	15444916	1
Caelo	4-hidroxibenzoato de metila	1601037-01	6
Caelo	4-hidroxibenzoato de metila	16256103	6
Caelo	4-hidroxibenzoato de metila	16256104	2
Caelo	4-hidroxibenzoato de metila	16256114	1
Caelo	4-hidroxibenzoato de metila	16256115	2
Caelo	4-hidroxibenzoato de metila	16256117	2
Caelo	4-hidroxibenzoato de metila	16256118	6
Caelo	4-hidroxibenzoato de metila	17158101	27
Caelo	4-hidroxibenzoato de metila	17343002	14
Caelo	4-hidroxibenzoato de metila	17343009	2
Caelo	4-hidroxibenzoato de metila	17343010	9
Caelo	4-hidroxibenzoato de metila	17343013	20
Caelo	4-hidroxibenzoato de metila	1807009-01	1
Caelo	4-hidroxibenzoato de metila	1816903	1
Caelo	4-hidroxibenzoato de metila	18176903	27
Caelo	4-hidroxibenzoato de metila	18176910	15
Caelo	4-hidroxibenzoato de metila	18176919	2
Caelo	4-hidroxibenzoato de metila	190672106	1
Caelo	4-hidroxibenzoato de metila	191302001	36
Caelo	4-hidroxibenzoato de metila	191302002	3
Caelo	4-hidroxibenzoato de metila	191302003	7
Caelo	4-hidroxibenzoato de metila	19130203	6
Caelo	4-hidroxibenzoato de metila	19130205	21
Caelo	4-hidroxibenzoato de metila	1913022001	1
Caelo	4-hidroxibenzoato de metila	19132001	1
Caelo	4-hidroxibenzoato de metila	2000388006	1
Caelo	4-hidroxibenzoato de metila	21000076005	18
Caelo	4-hidroxibenzoato de metila	21000076005n	1
Caelo	4-hidroxibenzoato de metila	21000076007	1
Caelo	4-hidroxibenzoato de metila	21000076011	17
Caelo	4-hidroxibenzoato de metila	21000076015	10
Caelo	4-hidroxibenzoato de metila	21000076017	1
Caelo	4-hidroxibenzoato de metila	22000388006	15
Caelo	4-hidroxibenzoato de metila	22000388009	2
Caelo	4-hidroxibenzoato de metila	22003498003	1
Caelo	4-hidroxibenzoato de metila	220830(22000388006)	1
Caelo	4-hidroxibenzoato de metila	22092002	1
Caelo	4-hidroxibenzoato de metila	290114PML01	1
Caelo	4-hidroxibenzoato de metila	6091402	1
Caelo	4-hidroxibenzoato de metila	713Q-01930	1
Caelo	4-hidroxibenzoato de metila	79/19	1
Caelo	4-hidroxibenzoato de metila	9011303	1
Caelo	4-hidroxibenzoato de metila	Caelo	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	22000388006	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	19130205	1
Caesar & Loretz GmbH/Gehe	4-hidroxibenzoato de metila	21000076015	1
Caesar & Loretz GmbH/Kehr	4-hidroxibenzoato de metila	191302003	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	191302001	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	18176903	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	191302003	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	19130203	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	21000076005	2
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	21000076005	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Sa	4-hidroxibenzoato de metila	19130205	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	21000076005	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de metila	21000076011	1
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	13268809	1
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	17158101	1
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	18176903	3
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	18176910	6
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	191302001	8
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	191302003	6
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	19130205	3
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	21000076005	9
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	21000076011	2
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	21000076015	4
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	220003388006	1
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	22000388006	6
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	22000388009	1
Caesar & Loretz GmbH	4-hidroxibenzoato de metila	22003498003	1
Caesar & Loretz Hild...	4-hidroxibenzoato de metila	191302003	1
Caesar & Loretz/Noweda	4-hidroxibenzoato de metila	191302001	1
Caesar & Loretz	4-hidroxibenzoato de metila	17343002	1
Caesar&loretz,Phoenix	4-hidroxibenzoato de metila	13268821	1
Caesar&Loretz	4-hidroxibenzoato de metila	17158101	1
Caesar/Noweda	4-hidroxibenzoato de metila	15063806	1
Cealo/Anzag	4-hidroxibenzoato de metila	19130205	1
Cealo/Gehe	4-hidroxibenzoato de metila	16256104	1
Eigenherstellung	4-hidroxibenzoato de metila		1
Eigenherstellung	4-hidroxibenzoato de metila	100912PML01	1
EuRho/ NOWEDA	4-hidroxibenzoato de metila	EA2781	1
EuRho	4-hidroxibenzoato de metila	110403101	1
Euro OTC	4-hidroxibenzoato de metila	1009022-01	1
Euro OTC	4-hidroxibenzoato de metila	1212011-01	1
Euro OTC	4-hidroxibenzoato de metila	1401027-01	1
Euro OTC	4-hidroxibenzoato de metila	1401027-02	2
Euro OTC	4-hidroxibenzoato de metila	140600501	1
Euro OTC	4-hidroxibenzoato de metila	1406005-01	2
Euro OTC	4-hidroxibenzoato de metila	1502009-01	11
Euro OTC	4-hidroxibenzoato de metila	1507042-01	10
Euro OTC	4-hidroxibenzoato de metila	1507042-02	4
Euro OTC	4-hidroxibenzoato de metila	1601037	1
Euro OTC	4-hidroxibenzoato de metila	1601037-01	5
Euro OTC	4-hidroxibenzoato de metila	1706005-01	9
Euro OTC	4-hidroxibenzoato de metila	1706005-02	3
Euro OTC	4-hidroxibenzoato de metila	170605-01	1
Euro OTC	4-hidroxibenzoato de metila	172620	1
Euro OTC	4-hidroxibenzoato de metila	1758101	1
Euro OTC	4-hidroxibenzoato de metila	1807009-01	28
Euro OTC	4-hidroxibenzoato de metila	1902025-01	3
Euro OTC	4-hidroxibenzoato de metila	19090009-01	1
Euro OTC	4-hidroxibenzoato de metila	1909009-01	8
Euro OTC	4-hidroxibenzoato de metila	2004013/01	1
Euro OTC	4-hidroxibenzoato de metila	200401301	2
Euro OTC	4-hidroxibenzoato de metila	2004013-01	5
Euro OTC	4-hidroxibenzoato de metila	2010001-01	3
Euro OTC	4-hidroxibenzoato de metila	2010001-02	5
Euro OTC	4-hidroxibenzoato de metila	2606022	1
Euro OTC	4-hidroxibenzoato de metila	2717M-01930	1
Euro OTC	4-hidroxibenzoato de metila	280903701	2
Euro OTC	4-hidroxibenzoato de metila	3115M-01930	1
Euro OTC	4-hidroxibenzoato de metila	3518A-01930	1
Euro OTC	4-hidroxibenzoato de metila	4312I-01930	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	4-hidroxibenzoato de metila	4314U-01930	1
Euro OTC	4-hidroxibenzoato de metila	EA2781	1
Euro/Phönix	4-hidroxibenzoato de metila	201000101	1
Fagron	4-hidroxibenzoato de metila		1
Fagron	4-hidroxibenzoato de metila	12D18-N01	1
Fagron	4-hidroxibenzoato de metila	12H02-N08	1
Fagron	4-hidroxibenzoato de metila	13B25-N03	2
Fagron	4-hidroxibenzoato de metila	13E27-N09	1
Fagron	4-hidroxibenzoato de metila	16256115	1
Fagron	4-hidroxibenzoato de metila	20111125-1	1
GATT-KOLLER/PHOENIX	4-hidroxibenzoato de metila	6112/01142814	1
Gatt-Koller	4-hidroxibenzoato de metila	1803308	1
Gehe	4-hidroxibenzoato de metila	11090020	1
Gehe	4-hidroxibenzoato de metila	11090031	1
Gehe	4-hidroxibenzoato de metila	15063818	1
Gehe	4-hidroxibenzoato de metila	17158101	1
Gehe	4-hidroxibenzoato de metila	1902025-01	1
Gehe	4-hidroxibenzoato de metila	2010001-02	1
Geibo	4-hidroxibenzoato de metila	22000388006	1
Hänseler	4-hidroxibenzoato de metila		2
Jenne	4-hidroxibenzoato de metila	21000076015	1
Kehr	4-hidroxibenzoato de metila	22003498003	1
L30	4-hidroxibenzoato de metila	17158101	2
Nachprüfung vom 31.1...	4-hidroxibenzoato de metila	12251624	2
Nachprüfung	4-hidroxibenzoato de metila	1718M-01930	1
Noweda/Caesar & Lore...	4-hidroxibenzoato de metila	22000388009	1
Noweda	4-hidroxibenzoato de metila	16256118	1
Noweda	4-hidroxibenzoato de metila	1706005-02	1
Noweda	4-hidroxibenzoato de metila	17158101	1
Noweda	4-hidroxibenzoato de metila	191302003	1
Phoenix	4-hidroxibenzoato de metila	1706005-01	1
Phoenix	4-hidroxibenzoato de metila	18176910	1
Phoenix	4-hidroxibenzoato de metila	200046011	1
Phoenix	4-hidroxibenzoato de metila	21000076011	1
Phoenix	4-hidroxibenzoato de metila	2100076007	1
Phoenix	4-hidroxibenzoato de metila	22000388009	1
Phoenix	4-hidroxibenzoato de metila	22003498003	1
Phönix 14.01.2014	4-hidroxibenzoato de metila	12251624	1
phönix 4.12.2013	4-hidroxibenzoato de metila	1212011/01	1
PHÖNIX	4-hidroxibenzoato de metila	15063819	1
Phönix	4-hidroxibenzoato de metila	16256103	1
Phönix	4-hidroxibenzoato de metila	17343010	1
Phönix	4-hidroxibenzoato de metila	1807009-01	1
Phönix	4-hidroxibenzoato de metila	191302001	1
Phönix	4-hidroxibenzoato de metila	2010001-01	2
Phönix	4-hidroxibenzoato de metila	2AKD3	1
sanacorb	4-hidroxibenzoato de metila	17343010	1
Sanacorp E.K :2,76...	4-hidroxibenzoato de metila	13268804	1

- 235 373 spectra from 1515 *Apo-Ident* customers from a total of 49 119 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *4-hidroxibenzoato de metila* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this

purpose, all relevant spectra of the various substances were compared with *4-hidroxibenzoato de metila* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	790	0	201 294
Type C	0	685	9	235 373

The substance/substance group *4-hidroxibenzoato de metila* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2405 %)
Type C	100.0000 % (> 99.9007 %)	98.7032 % (> 98.2709 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20693	22305	10,68	200,51
20697	22305	11,52	200,96
22305	22305	0,00	203,35
23223	22305	12,97	201,26
24223	24223	0,00	200,76
24588	22305	15,83	203,83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**4-hidroxibenzoato de propila**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20981-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

4-hidroxibenzoato de propila; Propylis parahydroxybenzoas

Special notes

When selecting the *4-hidroxibenzoato de propila* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
4-hidroxibenzoato de propila	5	3	73

Second-stage model

For differentiation of the substance/substance group *4-hidroxibenzoato de propila* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *4-hidroxibenzoato de propila* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	92,36	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *4-hidroxibenzoato de propila* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *4-hidroxibenzoato de propila*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	4-hidroxibenzoato de propila	11373523	20981	40	1402440
Caelo	4-hidroxibenzoato de propila	13365009	21758	60	20131203
Caelo	4-hidroxibenzoato de propila	162595	22754	40	20161005*
Caelo	4-hidroxibenzoato de propila	162595	22765	40	20161005*
Caelo	4-hidroxibenzoato de propila	190732	24497	40	20190404*
Caelo	4-hidroxibenzoato de propila	22002607	26367	40	20220930*
Caelo	4-hidroxibenzoato de propila	22002607	26367SI	20	20220930*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 7 reference samples from the substance/substance group *4-hidroxibenzoato de propila*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 682 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *4-hidroxibenzoato de propila*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	4-hidroxibenzoato de propila	171970	23675	40
Caelo	4-hidroxibenzoato de propila	23000158	26708	40
Gatt-Koller	4-hidroxibenzoato de propila	22J02745	27098	30
Caelo	4-hidroxibenzoato de propila	23000158	26708SI	20
Gatt-Koller	4-hidroxibenzoato de propila	22J02745	27098SI	20

- 201 934 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 322 spectra from 236 *Apo-Ident* customers from 76 batches from the substance/substance group *4-hidroxibenzoato de propila*.

- Among them are spectra of independent samples from 72 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	4-hidroxibenzoato de propila	191700004	1
	4-hidroxibenzoato de propila	191700004280622/1	1
	4-hidroxibenzoato de propila	21000901006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	4-hidroxibenzoato de propila	21000901013	1
	4-hidroxibenzoato de propila	23000158002	9
	4-hidroxibenzoato de propila	23000158005	3
AHD	4-hidroxibenzoato de propila	11373523	1
Anzag	4-hidroxibenzoato de propila	11373512	2
Caelo	4-hidroxibenzoato de propila		1
Caelo	4-hidroxibenzoato de propila	1108211931	1
Caelo	4-hidroxibenzoato de propila	11102609	1
Caelo	4-hidroxibenzoato de propila	11102611	2
Caelo	4-hidroxibenzoato de propila	11102624	1
Caelo	4-hidroxibenzoato de propila	11121709	1
Caelo	4-hidroxibenzoato de propila	113735	1
Caelo	4-hidroxibenzoato de propila	11373505	1
Caelo	4-hidroxibenzoato de propila	11373512	3
Caelo	4-hidroxibenzoato de propila	11373518	2
Caelo	4-hidroxibenzoato de propila	113735223	1
Caelo	4-hidroxibenzoato de propila	11373523	2
Caelo	4-hidroxibenzoato de propila	11373524	1
Caelo	4-hidroxibenzoato de propila	13051504	1
Caelo	4-hidroxibenzoato de propila	13100208	1
Caelo	4-hidroxibenzoato de propila	13100215	7
Caelo	4-hidroxibenzoato de propila	13100217	3
Caelo	4-hidroxibenzoato de propila	13100218	2
Caelo	4-hidroxibenzoato de propila	13100219	1
Caelo	4-hidroxibenzoato de propila	13365006	5
Caelo	4-hidroxibenzoato de propila	13365009	3
Caelo	4-hidroxibenzoato de propila	13365011	5
Caelo	4-hidroxibenzoato de propila	13365012	2
Caelo	4-hidroxibenzoato de propila	14359005	8
Caelo	4-hidroxibenzoato de propila	14359006	4
Caelo	4-hidroxibenzoato de propila	14359008	26
Caelo	4-hidroxibenzoato de propila	14359009	1
Caelo	4-hidroxibenzoato de propila	14359019	1
Caelo	4-hidroxibenzoato de propila	14359020	4
Caelo	4-hidroxibenzoato de propila	14359025	2
Caelo	4-hidroxibenzoato de propila	15246501	1
Caelo	4-hidroxibenzoato de propila	15246502	2
Caelo	4-hidroxibenzoato de propila	15276514	4
Caelo	4-hidroxibenzoato de propila	16259505	16
Caelo	4-hidroxibenzoato de propila	16259516	16
Caelo	4-hidroxibenzoato de propila	16259520	2
Caelo	4-hidroxibenzoato de propila	16359006	1
Caelo	4-hidroxibenzoato de propila	17343101	12
Caelo	4-hidroxibenzoato de propila	17343105	3
Caelo	4-hidroxibenzoato de propila	17343108	9
Caelo	4-hidroxibenzoato de propila	17343110	8
Caelo	4-hidroxibenzoato de propila	19073203	14
Caelo	4-hidroxibenzoato de propila	1913I-01931	1
Caelo	4-hidroxibenzoato de propila	191700002	1
Caelo	4-hidroxibenzoato de propila	191700004	33
Caelo	4-hidroxibenzoato de propila	191700007	1
Caelo	4-hidroxibenzoato de propila	191700009	3
Caelo	4-hidroxibenzoato de propila	19170004	1
Caelo	4-hidroxibenzoato de propila	21000601006	1
Caelo	4-hidroxibenzoato de propila	21000733001	1
Caelo	4-hidroxibenzoato de propila	21000733002	11
Caelo	4-hidroxibenzoato de propila	21000901006	2
Caelo	4-hidroxibenzoato de propila	220420	1
Caelo	4-hidroxibenzoato de propila	221014PAS01	1
Caelo	4-hidroxibenzoato de propila	23000158002	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	4-hidroxibenzoato de propila	290114PML03	1
Caelo	4-hidroxibenzoato de propila	3041408	1
Caelo	4-hidroxibenzoato de propila	3115M-01931	1
Caelo	4-hidroxibenzoato de propila	3217M-01931	1
Caelo	4-hidroxibenzoato de propila	4314U-01931	1
Caelo	4-hidroxibenzoato de propila	713Q-01931	1
Caelo	4-hidroxibenzoato de propila	82792159	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de propila	19073203	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de propila	19073203	1
Caesar & Loretz GmbH/GEHE	4-hidroxibenzoato de propila	17343108	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de propila	191700002	1
Caesar & Loretz GmbH...	4-hidroxibenzoato de propila	191700004	2
Caesar & Loretz GmbH...	4-hidroxibenzoato de propila	17343110	1
Caesar & Loretz GmbH	4-hidroxibenzoato de propila	191700004	12
Caesar & Loretz GmbH	4-hidroxibenzoato de propila	21000733002	1
Caesar & Loretz GmbH	4-hidroxibenzoato de propila	21000733005	1
Caesar & Loretz GmbH	4-hidroxibenzoato de propila	21000901006	1
Caesar & Loretz GmbH	4-hidroxibenzoato de propila	21000901013	1
Caesar & Loretz GmbHAnzag	4-hidroxibenzoato de propila	191700004	1
Caesar & Loretz	4-hidroxibenzoato de propila	15276514	1
Caesar &Loretz GmbH	4-hidroxibenzoato de propila	13100215	1
Caesar/Noweda	4-hidroxibenzoato de propila	3710M-01931	2
Carlo/Phönix/5,95	4-hidroxibenzoato de propila	19073203	1
Euro OTC	4-hidroxibenzoato de propila	2509025	1
Fagron	4-hidroxibenzoato de propila	12B13-N04	1
Fagron	4-hidroxibenzoato de propila	610M-01931	1
GATT-KOLLER/PHOENIX	4-hidroxibenzoato de propila	5080/11130214	1
Gatt-Koller	4-hidroxibenzoato de propila	1800302	1
Gehe 5.3.14	4-hidroxibenzoato de propila	13100215	1
Gehe	4-hidroxibenzoato de propila	16259505	1
Hänseler	4-hidroxibenzoato de propila		1
Kehr	4-hidroxibenzoato de propila	23000158002	1
Noweda	4-hidroxibenzoato de propila	11373505	1
Noweda	4-hidroxibenzoato de propila	14359005	1
Noweda	4-hidroxibenzoato de propila	14359020	1
Noweda	4-hidroxibenzoato de propila	17343101	1
Noweda	4-hidroxibenzoato de propila	17343105	1
PHOENIX 10.03.2014	4-hidroxibenzoato de propila	11373526	1
Phoenix	4-hidroxibenzoato de propila	13100215	1
Phoenix	4-hidroxibenzoato de propila	19073203	1
Phönix 14.01.2014	4-hidroxibenzoato de propila	11373526	1
Phönix	4-hidroxibenzoato de propila	17343108	1
Sanacorp	4-hidroxibenzoato de propila	16259505	1
Sanacorp	4-hidroxibenzoato de propila	16259516	1
Sanacorp	4-hidroxibenzoato de propila	191700004	1
Sanacorp	4-hidroxibenzoato de propila	23000158002	1
Sanacorp	4-hidroxibenzoato de propila	23000158005	1
Sanacorp	4-hidroxibenzoato de propila	AKD3	1
siehe WE-Prüfprotokoll	4-hidroxibenzoato de propila	84/11	1

- 235 745 spectra from 1515 *Apo-Ident* customers from a total of 49 185 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *4-hidroxibenzoato de propila* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *4-hidroxibenzoato de propila* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	150	0	201 934
Type C	0	319	3	235 745

The substance/substance group *4-hidroxibenzoato de propila* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.0683 % (> 98.1366 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20981	20981	0,00	174,36
21758	26367	11,12	167,75
22754	22754	0,00	184,77
22765	22765	0,00	181,06
24497	24497	0,00	191,42
26367	26367	0,00	181,91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de ciproterona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20593-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de ciproterona; Ciproterona, acetato; Cyproteroni acetas

Special notes

When selecting the *Acetato de ciproterona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de ciproterona	8	9	69

Second-stage model

For differentiation of the substance/substance group *Acetato de ciproterona* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de ciproterona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de prilocaína	66,32	–
⋮	⋮	⋮
Cloridrato de oxibutinina	>50	84,24
Prednicarbato	>50	100,38
Cloridrato de amitriptilina	>50	123,37
Capsaicina	>50	157,62
Levocarnitina	>50	160,01
Citrato de sódio	>50	205,52
Tetracaína	>50	206,95
Valina	>50	244,19
Metoxisaleno	>50	343,09
Acetato de noretisterona	>50	372,78
Cloridrato de quinina di-hidratado	>50	385,73
Alfaestradiol	>50	385,94
Piridoxal-5-fosfato	>50	467,07
Cloridrato de ciprofloxacina	>50	511,01
Heparina sódica	>50	627,00
Triclosan	>50	1531,72
Amifampridina	>50	2159,85
Sacarose	>50	2311,03

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de ciproterona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de ciproterona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Acetato de ciproterona	APCPA140201CP	23988	40	20140617
Audor Pharma	Acetato de ciproterona	APX03-181002-m0C	24814	40	20181213

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Acetato de ciproterona	1611003	22875	40	20161201*
Euro OTC	Acetato de ciproterona	1810017	24317	40	20181108*
Fagron	Acetato de ciproterona	13C11-N02	21262	40	1501534
Fagron	Acetato de ciproterona	13J16-No4	21985	75	1602654
Fagron	Acetato de ciproterona	15I11-B01-322117	22665	40	20150921
Fagron	Acetato de ciproterona	17D11-B07-333693	23238	40	20170501
Fagron	Acetato de ciproterona	17D11-B07-333693	23238SI	20	20170501

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 375 spectra of 9 reference samples from the substance/substance group *Acetato de ciproterona*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 587 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 771 spectra of 24 reference samples from the substance/substance group *Acetato de ciproterona*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Acetato de ciproterona	1903011	24609	40
Euro OTC	Acetato de ciproterona	1910022	24957	40
Euro OTC	Acetato de ciproterona	2003045	25270	40
Euro OTC	Acetato de ciproterona	2101023	25532	40
Euro OTC	Acetato de ciproterona	2205022	26192	40
Euro OTC	Acetato de ciproterona	2409015	27405	40
Fagron	Acetato de ciproterona	18G25-B02-352728	24289	40
Fagron	Acetato de ciproterona	22I13-B01-228645	26826	40
Fagron	Acetato de ciproterona	24A08-B08-235276	27178	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Acetato de ciproterona	APCPA140201CP	23988SI†	20
Audor Pharma	Acetato de ciproterona	APX03-181002-m0C	24814SI†	40
Euro OTC	Acetato de ciproterona	1611003	22875SI†	30
Euro OTC	Acetato de ciproterona	1810017	24317SI†	20
Euro OTC	Acetato de ciproterona	1903011	24609SI	20
Euro OTC	Acetato de ciproterona	1910022	24957SI	22
Euro OTC	Acetato de ciproterona	2003045	25270SI	30
Euro OTC	Acetato de ciproterona	2101023	25532SI	31
Euro OTC	Acetato de ciproterona	2205022	26192SI	32
Euro OTC	Acetato de ciproterona	2409015	27405SI	30
Fagron	Acetato de ciproterona	13J16-No4	21985SI†	23
Fagron	Acetato de ciproterona	15I11-B01-322117	22665SI†	33
Fagron	Acetato de ciproterona	18G25-B02-352728	24289SI	20
Fagron	Acetato de ciproterona	22I13-B01-228645	26826SI	30
Fagron	Acetato de ciproterona	24A08-B08-235276	27178SI	30

- 201 313 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 114 spectra from 65 *Apo-Ident* customers from 72 batches from the substance/substance group *Acetato de ciproterona*.
- Among them are spectra of independent samples from 69 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Audor Pharma	Acetato de ciproterona	APCPA140201CP	2
Audor Pharma	Acetato de ciproterona	APX03-181002-m0C	1
Audor Pharma	Acetato de ciproterona	cpa140201cp	1
Audor Pharma	Acetato de ciproterona	X03-181002-m0C	1
Caelo	Acetato de ciproterona	13j16-n04	1
Caelo	Acetato de ciproterona	17D11-B07-334581	3
Caelo	Acetato de ciproterona	18G25-B02-352728	1
Caelo	Acetato de ciproterona	CPA150301	1
Ebert-Jacobi	Acetato de ciproterona	16K09-B04-329036	1
Eu Rho/XX	Acetato de ciproterona	2003045-01	2
Euro OTC	Acetato de ciproterona	1502038-01	1
Euro OTC	Acetato de ciproterona	2003045-01	3
Euro OTC	Acetato de ciproterona	2101023-01	2
Fagron	Acetato de ciproterona	11L22-N02	1
Fagron	Acetato de ciproterona	12D02-N13	1
Fagron	Acetato de ciproterona	12F25-N09	3
Fagron	Acetato de ciproterona	12J24-N02	1
Fagron	Acetato de ciproterona	12L19-N05	3
Fagron	Acetato de ciproterona	13/09-N03	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Acetato de ciproterona	13/16-N04	2
Fagron	Acetato de ciproterona	13j16n04	1
Fagron	Acetato de ciproterona	13J16-N04	2
Fagron	Acetato de ciproterona	13j16-no4	1
Fagron	Acetato de ciproterona	15H04-B06-311064	1
Fagron	Acetato de ciproterona	15I11-B01-315381	2
Fagron	Acetato de ciproterona	16K09-B04-329037	1
Fagron	Acetato de ciproterona	17D11-B07	1
Fagron	Acetato de ciproterona	17D11-B07-336729	2
Fagron	Acetato de ciproterona	17D11-B07-338440	1
Fagron	Acetato de ciproterona	18041805	1
Fagron	Acetato de ciproterona	18B05_B05_346309	1
Fagron	Acetato de ciproterona	18B05-346308	1
Fagron	Acetato de ciproterona	18B05-B05-346307	1
Fagron	Acetato de ciproterona	18B05-B05-346309	3
Fagron	Acetato de ciproterona	18G25-B02	1
Fagron	Acetato de ciproterona	18G25-B02-352307	2
Fagron	Acetato de ciproterona	18G25-B02-352728	3
Fagron	Acetato de ciproterona	18G25-B02-354474	1
Fagron	Acetato de ciproterona	18G25-B02-354475	3
Fagron	Acetato de ciproterona	18G25-B02-354476	1
Fagron	Acetato de ciproterona	18G25-B02-355388	2
Fagron	Acetato de ciproterona	18G25-B02-358855	3
Fagron	Acetato de ciproterona	18G25-B02-358856	4
Fagron	Acetato de ciproterona	18G25-B02-358857	1
Fagron	Acetato de ciproterona	19A23-B04	2
Fagron	Acetato de ciproterona	19A23-B04_363300	1
Fagron	Acetato de ciproterona	19A23-B04-363299	1
Fagron	Acetato de ciproterona	19a23-b04-363300	1
Fagron	Acetato de ciproterona	19A23-B04-363300	2
Fagron	Acetato de ciproterona	19A23-B04-363301	1
Fagron	Acetato de ciproterona	19A23-B04-363302	1
Fagron	Acetato de ciproterona	19A23B04367910	1
Fagron	Acetato de ciproterona	19A23-B04367910	1
Fagron	Acetato de ciproterona	19A23-B04-367910	3
Fagron	Acetato de ciproterona	19A23-B04-363301	1
Fagron	Acetato de ciproterona	19A23-B04-367910	1
Fagron	Acetato de ciproterona	20101807	1
Fagron	Acetato de ciproterona	20K11-F01	1
Fagron	Acetato de ciproterona	20K11-F01-376805	1
Fagron	Acetato de ciproterona	20K11-F01-376807	1
Fagron	Acetato de ciproterona	21F22-B04-213628	4
Fagron	Acetato de ciproterona	21J12-B02-215671	1
Fagron	Acetato de ciproterona	21L17-B02	2
Fagron	Acetato de ciproterona	21L17-B02-217596	1
Fagron	Acetato de ciproterona	21L17-B02-217628	1
Fagron	Acetato de ciproterona	22113-B01-228645	1
Fagron	Acetato de ciproterona	2OK11-F01-376805	1
Fagron	Acetato de ciproterona	2OK11-FO1-376805	1
Fagron	Acetato de ciproterona	8B11-N06	1
Fagron	Acetato de ciproterona	B0392/110020	3
Fagron	Acetato de ciproterona	B04-3664709	1
Fagron	Acetato de ciproterona	EU-CPA-170301	1
Fargon/Noweda	Acetato de ciproterona	18G25-B02-352729	1
Fargon/Noweda	Acetato de ciproterona	18G25-B02-354476	1
Gehe	Acetato de ciproterona	22I13-B01-228645	1
Sanacorp	Acetato de ciproterona	18B05-B05-346307	1

- 235 953 spectra from 1515 *Apo-Ident* customers from a total of 49 186 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetato de ciproterona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetato de ciproterona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	375	0	152 587
Type B	0	771	0	201 313
Type C	0	114	0	235 953

The substance/substance group *Acetato de ciproterona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2218 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 94.7368 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21262	21262	0,00	109,91
21985	21985	0,00	110,79
22665	21985	2,72	115,03
22875	22875	0,00	112,37
23238	21985	3,72	109,72
23988	21985	2,56	109,74
24317	24317	0,00	110,75
24814	21985	3,97	112,70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de dexametasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20313-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de dexametasona; Dexametasona, acetato; Dexamethasoni acetas

Special notes

When selecting the *Acetato de dexametasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de dexametasona	7	3	116

Second-stage model

For differentiation of the substance/substance group *Acetato de dexametasona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de dexametasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	57,51	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de dexametasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de dexametasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetato de dexametasona	13260703	21301	40	1412430
Caelo	Acetato de dexametasona	13260706	21593	60	1502537
Caelo	Acetato de dexametasona	14200207	21815	60	20140807
Caelo	Acetato de dexametasona	14200207	21815SI	30	20140807
Caelo	Acetato de dexametasona	20002252	25448	40	2102142
Caelo	Acetato de dexametasona	20002252	25448SI	34	2102142
Caelo	Acetato de dexametasona	23000428	26942	40	20230907*
Caelo	Acetato de dexametasona	23000428	26942SI	40	20230907*
Euro OTC	Acetato de dexametasona	1405024-01	21614	60	20140620
Euro OTC	Acetato de dexametasona	1405024-01	21614SI	45	20140620
Euro OTC	Acetato de dexametasona	1708011	23693	40	20171002*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 489 spectra of 11 reference samples from the substance/substance group *Acetato de dexametasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 473 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 281 spectra of 8 reference samples from the substance/substance group *Acetato de dexametasona*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetato de dexametasona	161066	22437	60
Caelo	Acetato de dexametasona	181730	24253	40
Caelo	Acetato de dexametasona	191192	24734	40
Caelo	Acetato de dexametasona	14200207	21815SI†	15
Caelo	Acetato de dexametasona	161066	22437SI	42
Caelo	Acetato de dexametasona	181730	24253SI	20
Caelo	Acetato de dexametasona	191192	24734SI	40
Euro OTC	Acetato de dexametasona	1708011	23693SI†	24

- 201 803 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 528 spectra from 272 *Apo-Ident* customers from 120 batches from the substance/substance group *Acetato de dexametasona*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 116 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Acetato de dexametasona	20004529006	1
	Acetato de dexametasona	20004529009	1
	Acetato de dexametasona	20004529018	2
	Acetato de dexametasona	23000428005	1
AHD	Acetato de dexametasona	1405024-03	1
AHD	Acetato de dexametasona	18173002	1
Alliance	Acetato de dexametasona	20004529014	1
apomix	Acetato de dexametasona	1405024-03	1
Bombastus	Acetato de dexametasona	16106616	1
Caelo	Acetato de dexametasona	11093210	1
Caelo	Acetato de dexametasona	11093211	1
Caelo	Acetato de dexametasona	11093215	1
Caelo	Acetato de dexametasona	11093217	1
Caelo	Acetato de dexametasona	12021801	2
Caelo	Acetato de dexametasona	12021803	3
Caelo	Acetato de dexametasona	12021811	1
Caelo	Acetato de dexametasona	12021814	2
Caelo	Acetato de dexametasona	13100401	1
Caelo	Acetato de dexametasona	13100403	5
Caelo	Acetato de dexametasona	13100404	3
Caelo	Acetato de dexametasona	13100406	1
Caelo	Acetato de dexametasona	13100407	4
Caelo	Acetato de dexametasona	13100408	2
Caelo	Acetato de dexametasona	13260701	4
Caelo	Acetato de dexametasona	13260702	1
Caelo	Acetato de dexametasona	13260703	3
Caelo	Acetato de dexametasona	13260705	1
Caelo	Acetato de dexametasona	1405024-01	1
Caelo	Acetato de dexametasona	140502403	1
Caelo	Acetato de dexametasona	14200201	3
Caelo	Acetato de dexametasona	14200205	3
Caelo	Acetato de dexametasona	14200207	1
Caelo	Acetato de dexametasona	14200208	2
Caelo	Acetato de dexametasona	14379601	1
Caelo	Acetato de dexametasona	14379602	2
Caelo	Acetato de dexametasona	14379607	5
Caelo	Acetato de dexametasona	14379608	1
Caelo	Acetato de dexametasona	14379609	3
Caelo	Acetato de dexametasona	14379611	3
Caelo	Acetato de dexametasona	14379615	4
Caelo	Acetato de dexametasona	14379616	5
Caelo	Acetato de dexametasona	14379617	1
Caelo	Acetato de dexametasona	15243201	5
Caelo	Acetato de dexametasona	15243202	4
Caelo	Acetato de dexametasona	15243203	1
Caelo	Acetato de dexametasona	16106601	1
Caelo	Acetato de dexametasona	16106602	3
Caelo	Acetato de dexametasona	16106603	6
Caelo	Acetato de dexametasona	16106603/171025DM	1
Caelo	Acetato de dexametasona	16106604	2
Caelo	Acetato de dexametasona	16106607	4
Caelo	Acetato de dexametasona	16106608	5
Caelo	Acetato de dexametasona	16106609	1
Caelo	Acetato de dexametasona	16106610	2
Caelo	Acetato de dexametasona	16106611	2
Caelo	Acetato de dexametasona	16106612	2
Caelo	Acetato de dexametasona	16106613	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de dexametasona	16106615	2
Caelo	Acetato de dexametasona	16106616	8
Caelo	Acetato de dexametasona	161066165624	1
Caelo	Acetato de dexametasona	16106617	6
Caelo	Acetato de dexametasona	16106619	5
Caelo	Acetato de dexametasona	1610662	1
Caelo	Acetato de dexametasona	16106622	2
Caelo	Acetato de dexametasona	16106623	1
Caelo	Acetato de dexametasona	16106624	2
Caelo	Acetato de dexametasona	1708011-01	1
Caelo	Acetato de dexametasona	18041813	1
Caelo	Acetato de dexametasona	18173001	11
Caelo	Acetato de dexametasona	18173002	12
Caelo	Acetato de dexametasona	18173004	5
Caelo	Acetato de dexametasona	18173007	3
Caelo	Acetato de dexametasona	18173008	6
Caelo	Acetato de dexametasona	18173010	1
Caelo	Acetato de dexametasona	18173011	7
Caelo	Acetato de dexametasona	18173012	12
Caelo	Acetato de dexametasona	18173014	2
Caelo	Acetato de dexametasona	1873011	1
Caelo	Acetato de dexametasona	1911201	1
Caelo	Acetato de dexametasona	19119021	1
Caelo	Acetato de dexametasona	191192001	9
Caelo	Acetato de dexametasona	191192002	8
Caelo	Acetato de dexametasona	191192003	1
Caelo	Acetato de dexametasona	191192004	7
Caelo	Acetato de dexametasona	191192005	5
Caelo	Acetato de dexametasona	19119201	9
Caelo	Acetato de dexametasona	19119202	15
Caelo	Acetato de dexametasona	19119204	4
Caelo	Acetato de dexametasona	191192040	1
Caelo	Acetato de dexametasona	191192201	1
Caelo	Acetato de dexametasona	20002252001	7
Caelo	Acetato de dexametasona	200045290008	1
Caelo	Acetato de dexametasona	20004529001	10
Caelo	Acetato de dexametasona	20004529002	9
Caelo	Acetato de dexametasona	20004529003	11
Caelo	Acetato de dexametasona	20004529006	5
Caelo	Acetato de dexametasona	20004529008	6
Caelo	Acetato de dexametasona	20004529009	1
Caelo	Acetato de dexametasona	20004529010	4
Caelo	Acetato de dexametasona	20004529012	1
Caelo	Acetato de dexametasona	20004529014	1
Caelo	Acetato de dexametasona	20004529015	2
Caelo	Acetato de dexametasona	20004529016	2
Caelo	Acetato de dexametasona	20004529017	1
Caelo	Acetato de dexametasona	20004529018	1
Caelo	Acetato de dexametasona	20004529019	1
Caelo	Acetato de dexametasona	2004529003	1
Caelo	Acetato de dexametasona	2004529017	1
Caelo	Acetato de dexametasona	211118(20004529002)	1
Caelo	Acetato de dexametasona	22/AKD2	1
Caelo	Acetato de dexametasona	3913Q-01326	1
Caelo	Acetato de dexametasona	4113I-01326	1
Caelo	Acetato de dexametasona	5/AD1	1
Caelo	Acetato de dexametasona	50(18173001)	1
Caelo	Acetato de dexametasona	8173004	1
Caesar & Loretz GmbH...	Acetato de dexametasona	18173004	1
Caesar & Loretz GmbH...	Acetato de dexametasona	18173012	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Acetato de dexametasona	18173008	1
Caesar & Loretz GmbH...	Acetato de dexametasona	18173012	1
Caesar & Loretz GmbH/Gehe	Acetato de dexametasona	20004529001	1
Caesar & Loretz GmbH/Gehe	Acetato de dexametasona	20004529009	1
Caesar & Loretz GmbH...	Acetato de dexametasona	20004529001	2
Caesar & Loretz GmbH...	Acetato de dexametasona	20004529001	1
Caesar & Loretz GmbH...	Acetato de dexametasona	18173008	1
Caesar & Loretz GmbH...	Acetato de dexametasona	19119202	1
Caesar & Loretz GmbH...	Acetato de dexametasona	20004529015	1
Caesar & Loretz GmbH...	Acetato de dexametasona	19119202	2
Caesar & Loretz GmbH...	Acetato de dexametasona	18173011	1
Caesar & Loretz GmbH...	Acetato de dexametasona	19119202	1
Caesar & Loretz GmbH	Acetato de dexametasona	18173002	1
Caesar & Loretz GmbH	Acetato de dexametasona	18173007	2
Caesar & Loretz GmbH	Acetato de dexametasona	18173008	3
Caesar & Loretz GmbH	Acetato de dexametasona	18173010	1
Caesar & Loretz GmbH	Acetato de dexametasona	18173012	6
Caesar & Loretz GmbH	Acetato de dexametasona	191192001	7
Caesar & Loretz GmbH	Acetato de dexametasona	191192002	2
Caesar & Loretz GmbH	Acetato de dexametasona	191192004	5
Caesar & Loretz GmbH	Acetato de dexametasona	191192005	1
Caesar & Loretz GmbH	Acetato de dexametasona	19119202	2
Caesar & Loretz GmbH	Acetato de dexametasona	19119203	1
Caesar & Loretz GmbH	Acetato de dexametasona	20002252001	1
Caesar & Loretz GmbH	Acetato de dexametasona	20004529001	4
Caesar & Loretz GmbH	Acetato de dexametasona	20004529002	1
Caesar & Loretz GmbH	Acetato de dexametasona	20004529003	3
Caesar & Loretz GmbH	Acetato de dexametasona	20004529006	1
Caesar & Loretz GmbH	Acetato de dexametasona	20004529008	1
CAESAR & LORETZ GMBH	Acetato de dexametasona	20004529008	1
Caesar & Loretz GmbH	Acetato de dexametasona	20004529009	1
Caesar & Loretz GmbH	Acetato de dexametasona	20004529010	2
Caesar & Loretz GmbH	Acetato de dexametasona	20004529015	4
Caesar & Loretz Hilden	Acetato de dexametasona	19119202	1
Caesar und Loretz GmbH	Acetato de dexametasona	18173011	1
ERho	Acetato de dexametasona	1405024-02	1
EuRho/Jenne	Acetato de dexametasona	1708011-02	1
EuRho/Noweda	Acetato de dexametasona	1708011-01	2
Eurho/Sanacorp	Acetato de dexametasona	1708011-01	1
EuRho	Acetato de dexametasona	1110007-01	1
Euro OTC	Acetato de dexametasona	1110007-01	3
Euro OTC	Acetato de dexametasona	1110007-02	5
Euro OTC	Acetato de dexametasona	1110007-03	1
Euro OTC	Acetato de dexametasona	1405024	1
Euro OTC	Acetato de dexametasona	1405024-01	1
Euro OTC	Acetato de dexametasona	140502402	1
Euro OTC	Acetato de dexametasona	1405024-02	9
Euro OTC	Acetato de dexametasona	140502403	1
Euro OTC	Acetato de dexametasona	1405024-03	19
Euro OTC	Acetato de dexametasona	1405024-04	2
Euro OTC	Acetato de dexametasona	1708011-01	27
Euro OTC	Acetato de dexametasona	1708011-02	6
europharma	Acetato de dexametasona	1110007-01	1
Fagron	Acetato de dexametasona	1110007	1
Fagron	Acetato de dexametasona	1110007-01	1
Fagron	Acetato de dexametasona	14200207	1
Fagron	Acetato de dexametasona	18173002	1
Gehe	Acetato de dexametasona	16106609	1
Gehe	Acetato de dexametasona	16106613	1
Gehe	Acetato de dexametasona	16106619	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Acetato de dexametasona	1708011-01	1
Gehe	Acetato de dexametasona	18173007	1
Gehe	Acetato de dexametasona	18173012	1
gehe	Acetato de dexametasona	19119021	1
Noweda	Acetato de dexametasona	1110007-02	1
Noweda	Acetato de dexametasona	13100406	1
Noweda	Acetato de dexametasona	1708011-02	1
Noweda	Acetato de dexametasona	18173010	1
Noweda	Acetato de dexametasona	20004529015	1
Phoenix	Acetato de dexametasona	20004529018	1
Phoenix	Acetato de dexametasona	23000428005	1
Phönix	Acetato de dexametasona		1
Phönix	Acetato de dexametasona	16106603	1
Sanacorp	Acetato de dexametasona	14379611	1
Sanacorp	Acetato de dexametasona	16106613	1
Sanacorp	Acetato de dexametasona	1708011-01	1
Sanacorp	Acetato de dexametasona	1708011-02	1
Sanacorp	Acetato de dexametasona	29994529018	1
Sanofi Chimie/ Gehe	Acetato de dexametasona	18173004	1

- 235 539 spectra from 1515 *Apo-Ident* customers from a total of 49 140 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetato de dexametasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetato de dexametasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	489	0	152 473
Type B	0	281	0	201 803
Type C	0	496	32	235 539

The substance/substance group *Acetato de dexametasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7730 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8648 %)
Type C	100.0000 % (> 99.9007 %)	93.9394 % (> 93.3712 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21301	21301	0,00	154,26
21593	21593	0,00	155,90
21614	21301	8,00	156,41
21815	21593	12,63	154,96
23693	23693	0,00	163,63
25448	25448	0,00	197,57
26942	26942	0,00	230,31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de hidrocortisona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20010-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de hidrocortisona; Hidrocortisona, acetato; Hydrocortisoni acetas

Special notes

When selecting the *Acetato de hidrocortisona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de hidrocortisona	7	16	594

Second-stage model

For differentiation of the substance/substance group *Acetato de hidrocortisona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de hidrocortisona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	102,09	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de hidrocortisona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de hidrocortisona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetato de hidrocortisona	13291708	21462	60	20130926
Caelo	Acetato de hidrocortisona	182780	24392	40	20181210*
Euro OTC	Acetato de hidrocortisona	1209003-01	21295	40	20121108
Euro OTC	Acetato de hidrocortisona	1209003-01	21295SI	45	20121108
Euro OTC	Acetato de hidrocortisona	1508029	21889	60	20150902*
Euro OTC	Acetato de hidrocortisona	1508029	21889SI	44	20150902*
Euro OTC	Acetato de hidrocortisona	1604052	22564	40	20160525*
Fagron	Acetato de hidrocortisona	15A30-B09-307090	22241	60	20150226
Fagron	Acetato de hidrocortisona	18H07-B03-356259	24590	40	20180829

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 429 spectra of 9 reference samples from the substance/substance group *Acetato de hidrocortisona*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 533 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1296 spectra of 36 reference samples from the substance/substance group *Acetato de hidrocortisona*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetato de hidrocortisona	16238706	23115	40
Caelo	Acetato de hidrocortisona	170862	23328	40
Caelo	Acetato de hidrocortisona	21002415001	25924	40
Caelo	Acetato de hidrocortisona	21003553	25992	40
Caelo	Acetato de hidrocortisona	22002539	26363	40
Caelo	Acetato de hidrocortisona	23001089	26853	40
Caelo	Acetato de hidrocortisona	23003142	27133	40
Euro OTC	Acetato de hidrocortisona	1706021	23559	40
Euro OTC	Acetato de hidrocortisona	1805010	24130	40
Euro OTC	Acetato de hidrocortisona	1907011	24789	40
Euro OTC	Acetato de hidrocortisona	2004029	25331	40
Euro OTC	Acetato de hidrocortisona	2205004	26212	40
Euro OTC	Acetato de hidrocortisona	2306007	26883	40
Euro OTC	Acetato de hidrocortisona	2406005	27349	40
Fagron	Acetato de hidrocortisona	22A17-B07-216283	26138	40
Fagron	Acetato de hidrocortisona	23E18-B03-229951	27266	40
Caelo	Acetato de hidrocortisona	16238706	23115SI	20
Caelo	Acetato de hidrocortisona	170862	23328SI	21
Caelo	Acetato de hidrocortisona	182780	24392SI†	32
Caelo	Acetato de hidrocortisona	21002415001	25924SI	40
Caelo	Acetato de hidrocortisona	21003553	25992SI	35
Caelo	Acetato de hidrocortisona	22002539	26363SI	40
Caelo	Acetato de hidrocortisona	23001089	26853SI	40
Caelo	Acetato de hidrocortisona	23003142	27133SI	30
Euro OTC	Acetato de hidrocortisona	1604052	22564SI†	30
Euro OTC	Acetato de hidrocortisona	1706021	23559SI	30
Euro OTC	Acetato de hidrocortisona	1805010	24130SI	21
Euro OTC	Acetato de hidrocortisona	1907011	24789SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Acetato de hidrocortisona	2004029	25331SI	40
Euro OTC	Acetato de hidrocortisona	2205004	26212SI	20
Euro OTC	Acetato de hidrocortisona	2306007	26883SI	40
Euro OTC	Acetato de hidrocortisona	2406005	27349SI	40
Fagron	Acetato de hidrocortisona	15A30-B09-307090	22241SI[†]	24
Fagron	Acetato de hidrocortisona	18H07-B03-356259	24590SI[†]	33
Fagron	Acetato de hidrocortisona	22A17-B07-216283	26138SI	40
Fagron	Acetato de hidrocortisona	23E18-B03-229951	27266SI	40

- 200 788 spectra from a total of 4025 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5588 spectra from 1259 *Apo-Ident* customers from 613 batches from the substance/substance group *Acetato de hidrocortisona*.
- Among them are spectra of independent samples from 591 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Acetato de hidrocortisona	14043902	1
	Acetato de hidrocortisona	21002415010	1
	Acetato de hidrocortisona	21002415011	1
	Acetato de hidrocortisona	21002415013	2
	Acetato de hidrocortisona	21002415014	1
	Acetato de hidrocortisona	21002415015	1
	Acetato de hidrocortisona	21003553006	1
	Acetato de hidrocortisona	2100415014	1
	Acetato de hidrocortisona	22002539002	11
	Acetato de hidrocortisona	22002539003	2
	Acetato de hidrocortisona	22002539004	7
	Acetato de hidrocortisona	22002539008	7
	Acetato de hidrocortisona	22002539009	13
	Acetato de hidrocortisona	22002539010	14
	Acetato de hidrocortisona	22002539013	17
	Acetato de hidrocortisona	22002539014	8
	Acetato de hidrocortisona	22002539015	17
	Acetato de hidrocortisona	22002539016	1
	Acetato de hidrocortisona	22002539018	6
	Acetato de hidrocortisona	22002539019	10
	Acetato de hidrocortisona	2200253904	2
	Acetato de hidrocortisona	2202539004	1
	Acetato de hidrocortisona	2205004-01	3
	Acetato de hidrocortisona	22H11-B01-229287	2
	Acetato de hidrocortisona	22K21-B02-225805	2
	Acetato de hidrocortisona	23001089003	2
	Acetato de hidrocortisona	23001089004	3

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Acetato de hidrocortisona	23001089005	20
	Acetato de hidrocortisona	23001089006	11
	Acetato de hidrocortisona	23001089009	10
	Acetato de hidrocortisona	23003142003	5
	Acetato de hidrocortisona	2306007-01	2
	Acetato de hidrocortisona	333961	1
	Acetato de hidrocortisona	HD0125	1
AEP	Acetato de hidrocortisona	18278005	1
AEP	Acetato de hidrocortisona	18278020	4
AHD 07.03.2017 EK: 5,33	Acetato de hidrocortisona	16004407	1
AHD/Euro	Acetato de hidrocortisona	1706021-01	1
AHD/Euro	Acetato de hidrocortisona	1805010-01	1
AHD	Acetato de hidrocortisona	1205034-01	1
AHD	Acetato de hidrocortisona	13291707	1
AHD	Acetato de hidrocortisona	1706021-01	1
AHD	Acetato de hidrocortisona	17219704	1
AHD	Acetato de hidrocortisona	17219708	1
AHD	Acetato de hidrocortisona	21002415004	1
AHD	Acetato de hidrocortisona	22002539003	1
AHD	Acetato de hidrocortisona	22002539009	1
AHD	Acetato de hidrocortisona	22002539013	1
AHD	Acetato de hidrocortisona	22002539018	1
AHD	Acetato de hidrocortisona	23001089006	1
AHD;05,02,15; 12.48EUR	Acetato de hidrocortisona	14144805	1
Alliance Healthcare	Acetato de hidrocortisona	20004117001	2
Alliance Healthcare	Acetato de hidrocortisona	21002415011	1
Alliance Healthcare	Acetato de hidrocortisona	22002539010	1
Alliance/EurRho	Acetato de hidrocortisona	1907011-02	1
Alliance/EurRho	Acetato de hidrocortisona	2004029-01	2
Alliance	Acetato de hidrocortisona	1604052-01	1
Alliance	Acetato de hidrocortisona	2004029-02	1
Alliance	Acetato de hidrocortisona	21002415014	1
Alliance	Acetato de hidrocortisona	21003553007	2
Alliance	Acetato de hidrocortisona	22002539014	1
Allianz Healthcare	Acetato de hidrocortisona	18278005	1
Allianz Healthcare	Acetato de hidrocortisona	18278021	1
Allianz	Acetato de hidrocortisona	17219705	1
AMH Niemann/Sanacorp	Acetato de hidrocortisona	17219705	1
Anzag 20.12.17 5.28	Acetato de hidrocortisona	17219702	1
Anzag	Acetato de hidrocortisona	1112031-02	1
Anzag	Acetato de hidrocortisona	1209003-01	1
Anzag	Acetato de hidrocortisona	16238708	1
Anzag	Acetato de hidrocortisona	16238712	1
Anzag	Acetato de hidrocortisona	16238713	1
Anzag	Acetato de hidrocortisona	17086206	2
Anzag	Acetato de hidrocortisona	17219702	2
Anzag	Acetato de hidrocortisona	17219703	1
Anzag	Acetato de hidrocortisona	18278021	2
Anzag	Acetato de hidrocortisona	20004117001	1
Anzag	Acetato de hidrocortisona	22002539013	1
Anzag	Acetato de hidrocortisona	2205004-01	1
Apo-ident	Acetato de hidrocortisona	1805010-01	1
Apo-ident	Acetato de hidrocortisona	1907011-01	1
apomix	Acetato de hidrocortisona	1404017-02	1
apomix	Acetato de hidrocortisona	16095407	1
Bombastus	Acetato de hidrocortisona	123Validierung	1
Bombastus	Acetato de hidrocortisona	1505008-03	1
Bombastus	Acetato de hidrocortisona	15356903	1
Bombastus	Acetato de hidrocortisona	1604052-01	1
Bombastus	Acetato de hidrocortisona	2712M01718	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caeelo	Acetato de hidrocortisona	17086204	1
Caello/Anzag	Acetato de hidrocortisona	15067003	1
Caelo	Acetato de hidrocortisona		7
Caelo	Acetato de hidrocortisona	10024150042	1
Caelo	Acetato de hidrocortisona	10024150112	1
Caelo	Acetato de hidrocortisona	10301904	1
Caelo	Acetato de hidrocortisona	1061704	1
Caelo	Acetato de hidrocortisona	11098604	1
Caelo	Acetato de hidrocortisona	11098612	1
Caelo	Acetato de hidrocortisona	11098615	1
Caelo	Acetato de hidrocortisona	1112031-02	1
Caelo	Acetato de hidrocortisona	11263902	1
Caelo	Acetato de hidrocortisona	11263905	1
Caelo	Acetato de hidrocortisona	11263913	1
Caelo	Acetato de hidrocortisona	11263915	2
Caelo	Acetato de hidrocortisona	11263916	1
Caelo	Acetato de hidrocortisona	11263917	3
Caelo	Acetato de hidrocortisona	1130317	1
Caelo	Acetato de hidrocortisona	118107-3	1
Caelo	Acetato de hidrocortisona	12008402	2
Caelo	Acetato de hidrocortisona	12008405	4
Caelo	Acetato de hidrocortisona	12021502	1
Caelo	Acetato de hidrocortisona	1205034-01	3
Caelo	Acetato de hidrocortisona	1209003-01	6
Caelo	Acetato de hidrocortisona	12121801	1
Caelo	Acetato de hidrocortisona	1213M-01718	1
Caelo	Acetato de hidrocortisona	12182402	10
Caelo	Acetato de hidrocortisona	12182403	5
Caelo	Acetato de hidrocortisona	12182404	19
Caelo	Acetato de hidrocortisona	12182405	17
Caelo	Acetato de hidrocortisona	12182408	2
Caelo	Acetato de hidrocortisona	12183403	1
Caelo	Acetato de hidrocortisona	12330102	8
Caelo	Acetato de hidrocortisona	12330103	8
Caelo	Acetato de hidrocortisona	12330104	9
Caelo	Acetato de hidrocortisona	12330105	3
Caelo	Acetato de hidrocortisona	12330106	4
Caelo	Acetato de hidrocortisona	12330107	8
Caelo	Acetato de hidrocortisona	12330108	15
Caelo	Acetato de hidrocortisona	12330110	2
Caelo	Acetato de hidrocortisona	12330111	3
Caelo	Acetato de hidrocortisona	12330111-3507411061	1
Caelo	Acetato de hidrocortisona	12330112	13
Caelo	Acetato de hidrocortisona	12330113	1
Caelo	Acetato de hidrocortisona	12330114	1
Caelo	Acetato de hidrocortisona	12330116	10
Caelo	Acetato de hidrocortisona	13155302	8
Caelo	Acetato de hidrocortisona	13155303	9
Caelo	Acetato de hidrocortisona	13155304	5
Caelo	Acetato de hidrocortisona	13155306	5
Caelo	Acetato de hidrocortisona	13155307	2
Caelo	Acetato de hidrocortisona	13155308	8
Caelo	Acetato de hidrocortisona	131553080	1
Caelo	Acetato de hidrocortisona	13291701	1
Caelo	Acetato de hidrocortisona	13291704	4
Caelo	Acetato de hidrocortisona	13291705	4
Caelo	Acetato de hidrocortisona	13291706	10
Caelo	Acetato de hidrocortisona	13291707	14
Caelo	Acetato de hidrocortisona	13291708	7
Caelo	Acetato de hidrocortisona	13291709	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de hidrocortisona	13291711	7
Caelo	Acetato de hidrocortisona	1391704	1
Caelo	Acetato de hidrocortisona	1391706	1
Caelo	Acetato de hidrocortisona	13G09-N08	2
Caelo	Acetato de hidrocortisona	1403903	1
Caelo	Acetato de hidrocortisona	14043901	11
Caelo	Acetato de hidrocortisona	14043902	10
Caelo	Acetato de hidrocortisona	14043903	12
Caelo	Acetato de hidrocortisona	14043904	14
Caelo	Acetato de hidrocortisona	14043905	11
Caelo	Acetato de hidrocortisona	14043906	9
Caelo	Acetato de hidrocortisona	14043907	14
Caelo	Acetato de hidrocortisona	14043908	1
Caelo	Acetato de hidrocortisona	1406211718	1
Caelo	Acetato de hidrocortisona	14144802	1
Caelo	Acetato de hidrocortisona	14144803	9
Caelo	Acetato de hidrocortisona	14144804	6
Caelo	Acetato de hidrocortisona	14144805	21
Caelo	Acetato de hidrocortisona	14144806	15
Caelo	Acetato de hidrocortisona	14144807	6
Caelo	Acetato de hidrocortisona	1430102	1
Caelo	Acetato de hidrocortisona	1430140	1
Caelo	Acetato de hidrocortisona	14301401	15
Caelo	Acetato de hidrocortisona	14301402	8
Caelo	Acetato de hidrocortisona	14301403	6
Caelo	Acetato de hidrocortisona	14301404	7
Caelo	Acetato de hidrocortisona	14301405	24
Caelo	Acetato de hidrocortisona	14301406	18
Caelo	Acetato de hidrocortisona	14301407	17
Caelo	Acetato de hidrocortisona	14301408	8
Caelo	Acetato de hidrocortisona	14I16-B01-300292	1
Caelo	Acetato de hidrocortisona	1501035	1
Caelo	Acetato de hidrocortisona	1505008-01	6
Caelo	Acetato de hidrocortisona	15061006	1
Caelo	Acetato de hidrocortisona	15061207	1
Caelo	Acetato de hidrocortisona	15067003	13
Caelo	Acetato de hidrocortisona	15067004	26
Caelo	Acetato de hidrocortisona	15067005	18
Caelo	Acetato de hidrocortisona	15067006	13
Caelo	Acetato de hidrocortisona	15067010	3
Caelo	Acetato de hidrocortisona	15067011	8
Caelo	Acetato de hidrocortisona	15067013	11
Caelo	Acetato de hidrocortisona	1508029-01	4
Caelo	Acetato de hidrocortisona	15216204	3
Caelo	Acetato de hidrocortisona	15356901	17
Caelo	Acetato de hidrocortisona	15356902	20
Caelo	Acetato de hidrocortisona	15356903	23
Caelo	Acetato de hidrocortisona	15356904	8
Caelo	Acetato de hidrocortisona	1536902	1
Caelo	Acetato de hidrocortisona	15A07-B03-306545	1
Caelo	Acetato de hidrocortisona	15H24_B01-316480	1
Caelo	Acetato de hidrocortisona	15H24-B01-314236	2
Caelo	Acetato de hidrocortisona	1600406	1
Caelo	Acetato de hidrocortisona	160044003	1
Caelo	Acetato de hidrocortisona	16004402	19
Caelo	Acetato de hidrocortisona	16004403	9
Caelo	Acetato de hidrocortisona	16004404	1
Caelo	Acetato de hidrocortisona	16004405	13
Caelo	Acetato de hidrocortisona	16004406	27
Caelo	Acetato de hidrocortisona	16004407	23

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de hidrocortisona	16004408	22
Caelo	Acetato de hidrocortisona	160044402	1
Caelo	Acetato de hidrocortisona	1604052	1
Caelo	Acetato de hidrocortisona	1604052-01	6
Caelo	Acetato de hidrocortisona	1605410	1
Caelo	Acetato de hidrocortisona	160629HA	1
Caelo	Acetato de hidrocortisona	16095402	1
Caelo	Acetato de hidrocortisona	16095404	33
Caelo	Acetato de hidrocortisona	16095405	22
Caelo	Acetato de hidrocortisona	16095406	26
Caelo	Acetato de hidrocortisona	16095407	37
Caelo	Acetato de hidrocortisona	16095408	4
Caelo	Acetato de hidrocortisona	16095410	7
Caelo	Acetato de hidrocortisona	1623708	1
Caelo	Acetato de hidrocortisona	16238704	11
Caelo	Acetato de hidrocortisona	16238705	3
Caelo	Acetato de hidrocortisona	16238706	34
Caelo	Acetato de hidrocortisona	16238706-12517/2	1
Caelo	Acetato de hidrocortisona	16238707	15
Caelo	Acetato de hidrocortisona	16238708	25
Caelo	Acetato de hidrocortisona	16238708-200417/1	1
Caelo	Acetato de hidrocortisona	16238709	8
Caelo	Acetato de hidrocortisona	16238710	23
Caelo	Acetato de hidrocortisona	16238712	25
Caelo	Acetato de hidrocortisona	16238713	8
Caelo	Acetato de hidrocortisona	16238713-20170818Ma2	1
Caelo	Acetato de hidrocortisona	16238714	12
Caelo	Acetato de hidrocortisona	1623888704	1
Caelo	Acetato de hidrocortisona	163163055402	1
Caelo	Acetato de hidrocortisona	166004407	1
Caelo	Acetato de hidrocortisona	16C15-B04-321459	1
Caelo	Acetato de hidrocortisona	17011402	1
Caelo	Acetato de hidrocortisona	17053185	1
Caelo	Acetato de hidrocortisona	170602101	1
Caelo	Acetato de hidrocortisona	1706021-01	11
Caelo	Acetato de hidrocortisona	170804HA/1604052-01	1
Caelo	Acetato de hidrocortisona	170856206	1
Caelo	Acetato de hidrocortisona	17086202	1
Caelo	Acetato de hidrocortisona	170862024	1
Caelo	Acetato de hidrocortisona	17086203	18
Caelo	Acetato de hidrocortisona	17086204	27
Caelo	Acetato de hidrocortisona	17086205	28
Caelo	Acetato de hidrocortisona	17086205-20170818Ma3	1
Caelo	Acetato de hidrocortisona	17086206	11
Caelo	Acetato de hidrocortisona	17086207	4
Caelo	Acetato de hidrocortisona	17086209	2
Caelo	Acetato de hidrocortisona	17086211	10
Caelo	Acetato de hidrocortisona	17086212	3
Caelo	Acetato de hidrocortisona	17086221	1
Caelo	Acetato de hidrocortisona	171106HA/17086204	1
Caelo	Acetato de hidrocortisona	17142802	1
Caelo	Acetato de hidrocortisona	1721905	1
Caelo	Acetato de hidrocortisona	17219702	21
Caelo	Acetato de hidrocortisona	17219703	26
Caelo	Acetato de hidrocortisona	17219704	26
Caelo	Acetato de hidrocortisona	17219705	65
Caelo	Acetato de hidrocortisona	172197050	1
Caelo	Acetato de hidrocortisona	172197055662	1
Caelo	Acetato de hidrocortisona	17219706	31
Caelo	Acetato de hidrocortisona	17219707	49

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de hidrocortisona	17219708	47
Caelo	Acetato de hidrocortisona	172197085556	1
Caelo	Acetato de hidrocortisona	17219709	8
Caelo	Acetato de hidrocortisona	17219710	2
Caelo	Acetato de hidrocortisona	17219713	4
Caelo	Acetato de hidrocortisona	17219714	1
Caelo	Acetato de hidrocortisona	17358402	1
Caelo	Acetato de hidrocortisona	17358403	9
Caelo	Acetato de hidrocortisona	17358404	1
Caelo	Acetato de hidrocortisona	17L19-B04-348983	1
Caelo	Acetato de hidrocortisona	18011304	1
Caelo	Acetato de hidrocortisona	180219HA/17219707	1
Caelo	Acetato de hidrocortisona	1805010-01	1
Caelo	Acetato de hidrocortisona	181115181	1
Caelo	Acetato de hidrocortisona	18121710	1
Caelo	Acetato de hidrocortisona	18142802	16
Caelo	Acetato de hidrocortisona	18142803	13
Caelo	Acetato de hidrocortisona	18142804	39
Caelo	Acetato de hidrocortisona	18142805	45
Caelo	Acetato de hidrocortisona	18142805-H20181115Ma	1
Caelo	Acetato de hidrocortisona	18142806	42
Caelo	Acetato de hidrocortisona	18142807	26
Caelo	Acetato de hidrocortisona	18142808	21
Caelo	Acetato de hidrocortisona	181428087	1
Caelo	Acetato de hidrocortisona	18142809	21
Caelo	Acetato de hidrocortisona	18142810	2
Caelo	Acetato de hidrocortisona	18142811	18
Caelo	Acetato de hidrocortisona	18142812	23
Caelo	Acetato de hidrocortisona	18142814	1
Caelo	Acetato de hidrocortisona	18142815	18
Caelo	Acetato de hidrocortisona	18142904	1
Caelo	Acetato de hidrocortisona	181442805	1
Caelo	Acetato de hidrocortisona	1827006	1
Caelo	Acetato de hidrocortisona	1827015	1
Caelo	Acetato de hidrocortisona	18278003	22
Caelo	Acetato de hidrocortisona	18278004	39
Caelo	Acetato de hidrocortisona	18278005	59
Caelo	Acetato de hidrocortisona	18278006	29
Caelo	Acetato de hidrocortisona	18278007	24
Caelo	Acetato de hidrocortisona	18278008	23
Caelo	Acetato de hidrocortisona	18278010	36
Caelo	Acetato de hidrocortisona	18278011	1
Caelo	Acetato de hidrocortisona	18278014	23
Caelo	Acetato de hidrocortisona	18278015	33
Caelo	Acetato de hidrocortisona	18278016	30
Caelo	Acetato de hidrocortisona	18278017	5
Caelo	Acetato de hidrocortisona	18278018	20
Caelo	Acetato de hidrocortisona	18278019	22
Caelo	Acetato de hidrocortisona	18278020	24
Caelo	Acetato de hidrocortisona	18278021	22
Caelo	Acetato de hidrocortisona	18278021ma	1
Caelo	Acetato de hidrocortisona	1828007	1
Caelo	Acetato de hidrocortisona	1828014	1
Caelo	Acetato de hidrocortisona	187278005	1
Caelo	Acetato de hidrocortisona	18H07-B03-357240	2
Caelo	Acetato de hidrocortisona	190372703	1
Caelo	Acetato de hidrocortisona	1907011-02	1
Caelo	Acetato de hidrocortisona	190910209	1
Caelo	Acetato de hidrocortisona	1913807	1
Caelo	Acetato de hidrocortisona	191383001	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de hidrocortisona	191383004	19
Caelo	Acetato de hidrocortisona	19138301	24
Caelo	Acetato de hidrocortisona	19138302	18
Caelo	Acetato de hidrocortisona	19138303	1
Caelo	Acetato de hidrocortisona	19138304	29
Caelo	Acetato de hidrocortisona	19138305	29
Caelo	Acetato de hidrocortisona	19138306	1
Caelo	Acetato de hidrocortisona	19138307	43
Caelo	Acetato de hidrocortisona	19138308	8
Caelo	Acetato de hidrocortisona	1918304	1
Caelo	Acetato de hidrocortisona	192241005	2
Caelo	Acetato de hidrocortisona	192241008	1
Caelo	Acetato de hidrocortisona	1938305	1
Caelo	Acetato de hidrocortisona	19j10-f04-366276	1
Caelo	Acetato de hidrocortisona	19J10-F04-366276	1
Caelo	Acetato de hidrocortisona	200000978004	1
Caelo	Acetato de hidrocortisona	200000978007	1
Caelo	Acetato de hidrocortisona	200004117001	1
Caelo	Acetato de hidrocortisona	2000078008	1
Caelo	Acetato de hidrocortisona	20000977002	13
Caelo	Acetato de hidrocortisona	20000978003	1
Caelo	Acetato de hidrocortisona	20000978004	34
Caelo	Acetato de hidrocortisona	20000978005	28
Caelo	Acetato de hidrocortisona	20000978006	31
Caelo	Acetato de hidrocortisona	20000978007	23
Caelo	Acetato de hidrocortisona	20000978008	21
Caelo	Acetato de hidrocortisona	20000978009	12
Caelo	Acetato de hidrocortisona	20000978010	8
Caelo	Acetato de hidrocortisona	2000097808	1
Caelo	Acetato de hidrocortisona	200009978005	1
Caelo	Acetato de hidrocortisona	20001708003	1
Caelo	Acetato de hidrocortisona	200041117006	1
Caelo	Acetato de hidrocortisona	200041147001	1
Caelo	Acetato de hidrocortisona	20004117001	65
Caelo	Acetato de hidrocortisona	20004117004	15
Caelo	Acetato de hidrocortisona	20004117005	4
Caelo	Acetato de hidrocortisona	20004117006	18
Caelo	Acetato de hidrocortisona	20004117007	3
Caelo	Acetato de hidrocortisona	2000411701	1
Caelo	Acetato de hidrocortisona	200041176	1
Caelo	Acetato de hidrocortisona	2000417001	2
Caelo	Acetato de hidrocortisona	20004278002	22
Caelo	Acetato de hidrocortisona	20004278003	30
Caelo	Acetato de hidrocortisona	20004278004	54
Caelo	Acetato de hidrocortisona	20004278005	16
Caelo	Acetato de hidrocortisona	20004278006	8
Caelo	Acetato de hidrocortisona	20004278008	13
Caelo	Acetato de hidrocortisona	20004278009	8
Caelo	Acetato de hidrocortisona	2000427806	1
Caelo	Acetato de hidrocortisona	2000977002	1
Caelo	Acetato de hidrocortisona	2000978008	1
Caelo	Acetato de hidrocortisona	2004029-01	2
Caelo	Acetato de hidrocortisona	2004117001	2
Caelo	Acetato de hidrocortisona	2004117006	1
Caelo	Acetato de hidrocortisona	2004117007	2
Caelo	Acetato de hidrocortisona	2004278005	1
Caelo	Acetato de hidrocortisona	2004278008	1
Caelo	Acetato de hidrocortisona	200660707	1
Caelo	Acetato de hidrocortisona	20160727Ma2	1
Caelo	Acetato de hidrocortisona	2021803	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de hidrocortisona	2061401	1
Caelo	Acetato de hidrocortisona	2100215013	1
Caelo	Acetato de hidrocortisona	210024150002	1
Caelo	Acetato de hidrocortisona	21002415001	35
Caelo	Acetato de hidrocortisona	21002415002	27
Caelo	Acetato de hidrocortisona	21002415004	31
Caelo	Acetato de hidrocortisona	21002415005	7
Caelo	Acetato de hidrocortisona	21002415006	21
Caelo	Acetato de hidrocortisona	21002415007	1
Caelo	Acetato de hidrocortisona	21002415008	6
Caelo	Acetato de hidrocortisona	21002415009	18
Caelo	Acetato de hidrocortisona	21002415010	12
Caelo	Acetato de hidrocortisona	21002415011	35
Caelo	Acetato de hidrocortisona	21002415012	13
Caelo	Acetato de hidrocortisona	21002415014	15
Caelo	Acetato de hidrocortisona	21002415015	3
Caelo	Acetato de hidrocortisona	2100245011	1
Caelo	Acetato de hidrocortisona	21003093011	1
Caelo	Acetato de hidrocortisona	2100355	1
Caelo	Acetato de hidrocortisona	210035530004	1
Caelo	Acetato de hidrocortisona	21003553002	1
Caelo	Acetato de hidrocortisona	21003553003	4
Caelo	Acetato de hidrocortisona	21003553004	16
Caelo	Acetato de hidrocortisona	21003553005	17
Caelo	Acetato de hidrocortisona	21003553006	11
Caelo	Acetato de hidrocortisona	21003553007	11
Caelo	Acetato de hidrocortisona	21003553009	4
Caelo	Acetato de hidrocortisona	21003553010	3
Caelo	Acetato de hidrocortisona	2100415004	1
Caelo	Acetato de hidrocortisona	2100415009	1
Caelo	Acetato de hidrocortisona	2200253008	1
Caelo	Acetato de hidrocortisona	22002539	1
Caelo	Acetato de hidrocortisona	22002539002	10
Caelo	Acetato de hidrocortisona	22002539003	9
Caelo	Acetato de hidrocortisona	22002539004	2
Caelo	Acetato de hidrocortisona	22002539005	3
Caelo	Acetato de hidrocortisona	22002539008	6
Caelo	Acetato de hidrocortisona	22002539009	1
Caelo	Acetato de hidrocortisona	22002539010	6
Caelo	Acetato de hidrocortisona	22002539013	1
Caelo	Acetato de hidrocortisona	22002539014	2
Caelo	Acetato de hidrocortisona	22002539015	4
Caelo	Acetato de hidrocortisona	22002539018	1
Caelo	Acetato de hidrocortisona	22002539019	2
Caelo	Acetato de hidrocortisona	2202539003	1
Caelo	Acetato de hidrocortisona	2202539004	1
Caelo	Acetato de hidrocortisona	2202539008	1
Caelo	Acetato de hidrocortisona	23001089004	1
Caelo	Acetato de hidrocortisona	25(1805010-01)	1
Caelo	Acetato de hidrocortisona	25101201	1
Caelo	Acetato de hidrocortisona	2612M01718	1
Caelo	Acetato de hidrocortisona	27091307	1
Caelo	Acetato de hidrocortisona	27091403	1
Caelo	Acetato de hidrocortisona	2734	1
Caelo	Acetato de hidrocortisona	28071508	1
Caelo	Acetato de hidrocortisona	301115	1
Caelo	Acetato de hidrocortisona	3110491	1
Caelo	Acetato de hidrocortisona	3110516	1
Caelo	Acetato de hidrocortisona	3434	1
Caelo	Acetato de hidrocortisona	418M-01718	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de hidrocortisona	6071801	1
Caelo	Acetato de hidrocortisona	6101707	1
Caelo	Acetato de hidrocortisona	7051303	1
Caelo	Acetato de hidrocortisona	7082003	1
Caelo	Acetato de hidrocortisona	7086205	1
Caelo	Acetato de hidrocortisona	84280411	1
Caelo	Acetato de hidrocortisona	978004	1
Caelo	Acetato de hidrocortisona	Caelo	2
Caelo	Acetato de hidrocortisona	Caelo/20004117005	1
Caelo	Acetato de hidrocortisona	Hydc01122022	1
Caelo	Acetato de hidrocortisona	NCEHAC161003	1
Caelo	Acetato de hidrocortisona	test	1
Caeol/Noweda	Acetato de hidrocortisona	19138307	1
Caeol/Phoenix	Acetato de hidrocortisona	16004402	1
Caeol/Phönix	Acetato de hidrocortisona	17219708	1
Caeolo/Noweda	Acetato de hidrocortisona	13155303	1
Caeolo/Spangro	Acetato de hidrocortisona	20000978004	1
Caesar & Lorenz GmbH	Acetato de hidrocortisona	18278016	1
Caesar & Lorenz GmbH	Acetato de hidrocortisona	19138305	1
Caesar & Lorenz GmbH	Acetato de hidrocortisona	20000978007	1
Caesar & Loretz /Alliance	Acetato de hidrocortisona	21002415010	2
Caesar & Loretz GmbH…	Acetato de hidrocortisona	14144806	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	19138308	4
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004117005	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415006	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415008	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415013	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	18278014	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21003553006	2
Caesar & Loretz GmbH…	Acetato de hidrocortisona	18278020	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004278003	2
Caesar & Loretz GmbH, Now	Acetato de hidrocortisona	22002539002	1
Caesar & Loretz GmbH/ AEP	Acetato de hidrocortisona	19138305	1
Caesar & Loretz GmbH/ AHD	Acetato de hidrocortisona	20000978010	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415011	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004117006	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004278004	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21003553006	2
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21003553009	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415011	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21003553004	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	18278004	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004278004	2
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004278006	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415011	3
Caesar & Loretz GmbH…	Acetato de hidrocortisona	20004117001	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415004	1
Caesar & Loretz GmbH/AEP	Acetato de hidrocortisona	18278014	1
Caesar & Loretz GmbH/AEP	Acetato de hidrocortisona	21002415001	1
Caesar & Loretz GmbH/AHD	Acetato de hidrocortisona	20004278003	1
Caesar & Loretz GmbH/AHD	Acetato de hidrocortisona	21002415001	1
Caesar & Loretz GmbH/AHD	Acetato de hidrocortisona	21002415011	2
Caesar & Loretz GmbH/AHD	Acetato de hidrocortisona	21002415014	2
Caesar & Loretz GmbH/AHD	Acetato de hidrocortisona	22002539004	3
Caesar & Loretz GmbH/all	Acetato de hidrocortisona	20000978005	1
Caesar & Loretz GmbH/Alli	Acetato de hidrocortisona	20000978004	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	191383001	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	19138307	1
Caesar & Loretz GmbH…	Acetato de hidrocortisona	21002415006	2
Caesar & Loretz GmbH…	Acetato de hidrocortisona	19138304	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004117001	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978007	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004278004	1
Caesar & Loretz GmbH/G	Acetato de hidrocortisona	20000978009	1
Caesar & Loretz GmbH/G	Acetato de hidrocortisona	21002415001	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	20000978006	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	20004117001	1
Caesar & Loretz GmbH/GEHE	Acetato de hidrocortisona	20004117001	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	20004117006	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	20004117007	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	20004278004	3
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	21002415001	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	21002415014	1
Caesar & Loretz GmbH/Gehe	Acetato de hidrocortisona	23001089005	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000977002	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004117004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004278002	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415014	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21003553006	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	22002539004	1
Caesar & Loretz GmbH/GEJE	Acetato de hidrocortisona	19138302	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978005	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415002	3
Caesar & Loretz GmbH...	Acetato de hidrocortisona	18278014	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	18278021	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000977002	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978006	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415006	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415011	1
Caesar & Loretz GmbH/K	Acetato de hidrocortisona	18278015	1
Caesar & Loretz GmbH/K	Acetato de hidrocortisona	19138301	1
Caesar & Loretz GmbH/K	Acetato de hidrocortisona	20004278003	1
Caesar & Loretz GmbH/Kehr	Acetato de hidrocortisona	18278016	1
Caesar & Loretz GmbH/Kehr	Acetato de hidrocortisona	191383001	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978009	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004278003	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415001	1
Caesar & Loretz GmbH/Now	Acetato de hidrocortisona	20004278006	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	18278017	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415001	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415002	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415006	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415014	3
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21003553009	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	191383004	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	191383001	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004117005	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004278004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415011	4
Caesar & Loretz GmbH...	Acetato de hidrocortisona	18142806	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	18278005	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	191383004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	19138301	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	19138304	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978006	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004278004	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415002	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415006	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415014	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21003553006	2
Caesar & Loretz GmbH...	Acetato de hidrocortisona	22002539004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	22002539005	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	22002539013	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	19138305	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	19138307	3
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978005	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978006	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20000978007	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	20004117001	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415002	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415008	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21002415010	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21003553004	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	21003553009	1
Caesar & Loretz GmbH...	Acetato de hidrocortisona	22002539003	1
Caesar & Loretz GmbH	Acetato de hidrocortisona		1
Caesar & Loretz GmbH	Acetato de hidrocortisona	12182405	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	15067004	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	16004402	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	16004408	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	16095405	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	16095406	2
Caesar & Loretz GmbH	Acetato de hidrocortisona	17219706	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	17219708	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	18142804	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	18142815	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	182778014	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278003	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278004	9
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278005	11
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278006	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278007	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278008	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278010	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278014	9
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278015	11
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278016	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278018	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278019	5
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278020	5
Caesar & Loretz GmbH	Acetato de hidrocortisona	18278021	7
Caesar & Loretz GmbH	Acetato de hidrocortisona	191383001	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	191383004	5
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138301	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138302	4
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138303	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138304	9
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138305	8
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138307	11
Caesar & Loretz GmbH	Acetato de hidrocortisona	19138308	2
Caesar & Loretz GmbH	Acetato de hidrocortisona	19A24	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000977002	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978004	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978005	9
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978006	8
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978007	12
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978008	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978009	4
Caesar & Loretz GmbH	Acetato de hidrocortisona	20000978010	4
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004117001	25
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004117004	6
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004117005	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004117006	5
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004117007	5
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278002	9
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278003	15
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278004	15
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278005	2
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278006	9
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278008	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	20004278009	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415001	16
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415002	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415004	4
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415005	6
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415006	7
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415008	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415009	2
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415010	10
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415011	14
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415012	7
Caesar & Loretz GmbH	Acetato de hidrocortisona	21002415014	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553002	1
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553004	2
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553005	6
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553006	7
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553007	6
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553009	4
Caesar & Loretz GmbH	Acetato de hidrocortisona	21003553010	4
Caesar & Loretz GmbH	Acetato de hidrocortisona	22002539002	6
Caesar & Loretz GmbH	Acetato de hidrocortisona	22002539003	5
Caesar & Loretz GmbH	Acetato de hidrocortisona	22002539004	3
Caesar & Loretz GmbH	Acetato de hidrocortisona	22002539008	6
Caesar & Loretz GmbH	Acetato de hidrocortisona	22002539019	2
Caesar & Loretz GmbH	Acetato de hidrocortisona	23001089005	1
Caesar & Loretz GmbHAnzag	Acetato de hidrocortisona	18278019	1
Caesar & Loretz Hild…	Acetato de hidrocortisona	20000978004	1
Caesar & Loretz Hilden	Acetato de hidrocortisona	18278005	1
Caesar & Loretz Hilden	Acetato de hidrocortisona	19138307	1
Caesar & Loretz Hilden	Acetato de hidrocortisona	20004278005	1
Caesar & Loretz/AHD	Acetato de hidrocortisona	17219706	1
Caesar & Loretz/Geil…	Acetato de hidrocortisona	20000978008	1
Caesar & Loretz/Geil…	Acetato de hidrocortisona	20004278004	2
Caesar & Loretz	Acetato de hidrocortisona	16095404	1
Caesar & Loretz	Acetato de hidrocortisona	17086203	1
Caesar & Loretz	Acetato de hidrocortisona	18142815	2
Caesar / Gehe	Acetato de hidrocortisona	15067003	1
Caesar u Loretz	Acetato de hidrocortisona	15067003	1
Caesar und Loretz GmbH	Acetato de hidrocortisona	18278020	1
Caesar&Loretz GmbH,P…	Acetato de hidrocortisona	16238708	1
Caesar&Loretz GmbH/AHD	Acetato de hidrocortisona	15356903	1
Caesar&Loretz GmbH/Anzag	Acetato de hidrocortisona	14301405	2
Caesar&Loretz GmbH	Acetato de hidrocortisona	21002415002	1
Caesar&loretz,Phoenix	Acetato de hidrocortisona	12182405	1
Caesar&loretz,Phoenix	Acetato de hidrocortisona	12330103	1
caesar&loretz,PHönix…	Acetato de hidrocortisona	15067003	1
Caesar&LoretzGmbH, P…	Acetato de hidrocortisona	18278006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar/Gehe	Acetato de hidrocortisona	20000978005	1
caesar	Acetato de hidrocortisona	14301402	1
Caolo	Acetato de hidrocortisona	17219707	2
Carli/ Phoenix	Acetato de hidrocortisona	20004117004	1
Cealo / Noweda	Acetato de hidrocortisona	13291707	1
Cealo, GEHE	Acetato de hidrocortisona	20004278002	2
Cealo/ Anzag	Acetato de hidrocortisona	16238712	1
Cealo/ Anzag	Acetato de hidrocortisona	17219702	1
Cealo/ Noweda	Acetato de hidrocortisona	20000978008	1
Cealo/Gehe	Acetato de hidrocortisona	16095410	2
Cealo/Noweda	Acetato de hidrocortisona	18278016	2
Cealo/Sanacorp	Acetato de hidrocortisona	20000978009	1
Cealo	Acetato de hidrocortisona	1706021-01	1
Eplus	Acetato de hidrocortisona	17219708	1
EuRho Noweda	Acetato de hidrocortisona	1907011-02	1
EuRho/ Anzag	Acetato de hidrocortisona	29(1907011-01)	1
Eurho/ Noweda	Acetato de hidrocortisona	1703021-01	1
EuRho/ NOWEDA	Acetato de hidrocortisona	1805010-01	2
EuRho/ VDL	Acetato de hidrocortisona	1706021-01	1
EuRho/AHD	Acetato de hidrocortisona	1706021-01	1
EuRho/Alliance Healt	Acetato de hidrocortisona	1907011-01	1
EuRho/Gehe	Acetato de hidrocortisona	1805010-01	2
EuRho/Kehr	Acetato de hidrocortisona	1907011-02	1
Eurho/Noweda	Acetato de hidrocortisona	200402902	1
EuRho/Phoenix	Acetato de hidrocortisona	1209003-01	1
EuRho/Phönix	Acetato de hidrocortisona	2004029-01	1
EuRho	Acetato de hidrocortisona	1107004-03	1
Eurho	Acetato de hidrocortisona	1706021-01	1
EuRho	Acetato de hidrocortisona	1706021-01	1
EuRho	Acetato de hidrocortisona	17086212	1
EuRho	Acetato de hidrocortisona	1805010-01	7
EuRho	Acetato de hidrocortisona	1907011-01	1
EuRho	Acetato de hidrocortisona	1907011-02	2
EuRho	Acetato de hidrocortisona	2004029-01	3
Euro OT/Anzag	Acetato de hidrocortisona	1706021-01	2
Euro OTC	Acetato de hidrocortisona		1
Euro OTC	Acetato de hidrocortisona	1107004-03	2
Euro OTC	Acetato de hidrocortisona	1112031-01	11
Euro OTC	Acetato de hidrocortisona	1112031-02	3
Euro OTC	Acetato de hidrocortisona	120503401	3
Euro OTC	Acetato de hidrocortisona	1205034-01	26
Euro OTC	Acetato de hidrocortisona	12090003-01	3
Euro OTC	Acetato de hidrocortisona	120900301	2
Euro OTC	Acetato de hidrocortisona	1209003-01	20
Euro OTC	Acetato de hidrocortisona	1404017-01	13
Euro OTC	Acetato de hidrocortisona	1404017-02	6
Euro OTC	Acetato de hidrocortisona	1404017-03	1
Euro OTC	Acetato de hidrocortisona	140900501	1
Euro OTC	Acetato de hidrocortisona	1409005-01	17
Euro OTC	Acetato de hidrocortisona	140900502	1
Euro OTC	Acetato de hidrocortisona	1409005-02	4
Euro OTC	Acetato de hidrocortisona	14301406	1
Euro OTC	Acetato de hidrocortisona	1500829-01	1
Euro OTC	Acetato de hidrocortisona	150103501	3
Euro OTC	Acetato de hidrocortisona	1501035-01	14
Euro OTC	Acetato de hidrocortisona	1502000801	1
Euro OTC	Acetato de hidrocortisona	1505008	1
Euro OTC	Acetato de hidrocortisona	150500801	3
Euro OTC	Acetato de hidrocortisona	1505008-01	54
Euro OTC	Acetato de hidrocortisona	1508023-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Acetato de hidrocortisona	1508029	2
Euro OTC	Acetato de hidrocortisona	150802901	1
Euro OTC	Acetato de hidrocortisona	1508029-01	36
Euro OTC	Acetato de hidrocortisona	1508029-02	4
Euro OTC	Acetato de hidrocortisona	1508029-03	1
Euro OTC	Acetato de hidrocortisona	15356903	1
Euro OTC	Acetato de hidrocortisona	16004406	2
Euro OTC	Acetato de hidrocortisona	160405201	5
Euro OTC	Acetato de hidrocortisona	1604052-01	77
Euro OTC	Acetato de hidrocortisona	16238707	1
Euro OTC	Acetato de hidrocortisona	170602-01	1
Euro OTC	Acetato de hidrocortisona	1706021	1
Euro OTC	Acetato de hidrocortisona	1706021-0	1
Euro OTC	Acetato de hidrocortisona	170602101	1
Euro OTC	Acetato de hidrocortisona	1706021-01	84
Euro OTC	Acetato de hidrocortisona	17066021-01	1
Euro OTC	Acetato de hidrocortisona	170830HA/1706021-01	1
Euro OTC	Acetato de hidrocortisona	17086202	1
Euro OTC	Acetato de hidrocortisona	17086203	1
Euro OTC	Acetato de hidrocortisona	17086204	1
Euro OTC	Acetato de hidrocortisona	17219705	1
Euro OTC	Acetato de hidrocortisona	17219709	1
Euro OTC	Acetato de hidrocortisona	180501001	8
Euro OTC	Acetato de hidrocortisona	1805010-01	123
Euro OTC	Acetato de hidrocortisona	18050101	1
Euro OTC	Acetato de hidrocortisona	1805010-1	1
Euro OTC	Acetato de hidrocortisona	18050101-01	1
Euro OTC	Acetato de hidrocortisona	180510-01	2
Euro OTC	Acetato de hidrocortisona	18142805	1
Euro OTC	Acetato de hidrocortisona	18142808	1
Euro OTC	Acetato de hidrocortisona	18142811	3
Euro OTC	Acetato de hidrocortisona	18278014	1
Euro OTC	Acetato de hidrocortisona	1907001-01	1
Euro OTC	Acetato de hidrocortisona	1907011	1
Euro OTC	Acetato de hidrocortisona	190701101	2
Euro OTC	Acetato de hidrocortisona	1907011-01	30
Euro OTC	Acetato de hidrocortisona	190701102	2
Euro OTC	Acetato de hidrocortisona	1907011-02	27
Euro OTC	Acetato de hidrocortisona	1907011-03	8
Euro OTC	Acetato de hidrocortisona	19070111-03	1
Euro OTC	Acetato de hidrocortisona	1907011-42	1
Euro OTC	Acetato de hidrocortisona	1907077-02	1
Euro OTC	Acetato de hidrocortisona	19138307	1
Euro OTC	Acetato de hidrocortisona	2004029	4
Euro OTC	Acetato de hidrocortisona	200402901	1
Euro OTC	Acetato de hidrocortisona	2004029-01	52
Euro OTC	Acetato de hidrocortisona	2004029-02	10
Euro OTC	Acetato de hidrocortisona	2205004_01	1
Euro OTC	Acetato de hidrocortisona	2205004-01	18
Euro OTC	Acetato de hidrocortisona	2604052-01	1
Euro OTC	Acetato de hidrocortisona	30(1805010-01)	1
Euro OTC	Acetato de hidrocortisona	31(1907011-01)	1
Euro OTC	Acetato de hidrocortisona	508029-01	2
Euro OTC	Acetato de hidrocortisona	911I-01718	1
Euro OTC	Acetato de hidrocortisona	EuroOTC	2
Euro OTC	Acetato de hidrocortisona	HCAZ11004K	1
Euro OTC	Acetato de hidrocortisona	K061828180402	1
Euro OTC	Acetato de hidrocortisona	L68934	1
Euro/ Sanacorp	Acetato de hidrocortisona	1409005-01	1
Euro/Alliance Healthcare	Acetato de hidrocortisona	1508029-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Gehe	Acetato de hidrocortisona	1404017-01	1
Euro/L10	Acetato de hidrocortisona	190701101	1
Euro/L10	Acetato de hidrocortisona	1907011-01	1
Euro/Noweda	Acetato de hidrocortisona	1805010-01	2
Euro/Phönix	Acetato de hidrocortisona	1805010	1
Euro/sanacorp	Acetato de hidrocortisona	1604052-01	1
Euro/Sanacorp	Acetato de hidrocortisona	1805010-01	1
Euroo/Noweda	Acetato de hidrocortisona	2004029-01	1
Europh-Gehe	Acetato de hidrocortisona	1508029-01	1
EuRro/Anzag	Acetato de hidrocortisona	1706021-01	2
Fagro/Gehe	Acetato de hidrocortisona	15A07-B03_306545	1
Fagro/Noweda	Acetato de hidrocortisona	18142804	1
Fagron	Acetato de hidrocortisona		1
Fagron	Acetato de hidrocortisona	11/01-N05	1
Fagron	Acetato de hidrocortisona	1112031	1
Fagron	Acetato de hidrocortisona	12330107	1
Fagron	Acetato de hidrocortisona	12K15-N04	6
Fagron	Acetato de hidrocortisona	13/31-B07-290061	1
Fagron	Acetato de hidrocortisona	13155311	1
Fagron	Acetato de hidrocortisona	13A03-N04	4
Fagron	Acetato de hidrocortisona	13B25-N04	2
Fagron	Acetato de hidrocortisona	13E31-N02	3
Fagron	Acetato de hidrocortisona	13E31-No2	1
Fagron	Acetato de hidrocortisona	13F25-B05-300290	2
Fagron	Acetato de hidrocortisona	13G09-N08	4
Fagron	Acetato de hidrocortisona	13J31-B07	3
Fagron	Acetato de hidrocortisona	13J31B07290061	1
Fagron	Acetato de hidrocortisona	13J31-B07-290061	2
Fagron	Acetato de hidrocortisona	13J31-B07-290062	2
Fagron	Acetato de hidrocortisona	14043903	1
Fagron	Acetato de hidrocortisona	14043905	1
Fagron	Acetato de hidrocortisona	14043906	1
Fagron	Acetato de hidrocortisona	14144804	1
Fagron	Acetato de hidrocortisona	14301402	1
Fagron	Acetato de hidrocortisona	14301408	1
Fagron	Acetato de hidrocortisona	14A13-B04	1
Fagron	Acetato de hidrocortisona	14A13-B04-294158	2
Fagron	Acetato de hidrocortisona	14I16-B01-300292	2
Fagron	Acetato de hidrocortisona	15067006	1
Fagron	Acetato de hidrocortisona	157000-0002	1
Fagron	Acetato de hidrocortisona	15A03-B09-307133	1
Fagron	Acetato de hidrocortisona	15A03-B09-307300	1
Fagron	Acetato de hidrocortisona	15A07-B03-306545	1
Fagron	Acetato de hidrocortisona	15A30-B09	1
Fagron	Acetato de hidrocortisona	15A30-B09-307133	4
Fagron	Acetato de hidrocortisona	15H24-B01	1
Fagron	Acetato de hidrocortisona	15h24-b01-314236	1
Fagron	Acetato de hidrocortisona	15H24-B01-314236	1
Fagron	Acetato de hidrocortisona	15H24-B01-316480	1
Fagron	Acetato de hidrocortisona	15I28-B12-316481	1
Fagron	Acetato de hidrocortisona	15J28-B12	1
Fagron	Acetato de hidrocortisona	15J28-B12-316481	1
Fagron	Acetato de hidrocortisona	15J28-b12-317771	1
Fagron	Acetato de hidrocortisona	15J28-B12-317771	1
Fagron	Acetato de hidrocortisona	16004402	1
Fagron	Acetato de hidrocortisona	160405201	1
Fagron	Acetato de hidrocortisona	1604052-01	1
Fagron	Acetato de hidrocortisona	16095407	2
Fagron	Acetato de hidrocortisona	16238707	1
Fagron	Acetato de hidrocortisona	16B03-B04	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Acetato de hidrocortisona	16B03-B04-319407	1
Fagron	Acetato de hidrocortisona	16B03-B04-320156	1
Fagron	Acetato de hidrocortisona	16C15-B04-321458	3
Fagron	Acetato de hidrocortisona	16C15-B04-321459	1
Fagron	Acetato de hidrocortisona	16H18-B04	2
Fagron	Acetato de hidrocortisona	16H18-B04-325093	3
Fagron	Acetato de hidrocortisona	16H18B04327324	1
Fagron	Acetato de hidrocortisona	16H18-B04-327324	1
Fagron	Acetato de hidrocortisona	16h18-b04-327325	1
Fagron	Acetato de hidrocortisona	16H18-B04-327325	2
Fagron	Acetato de hidrocortisona	16J28-B05	1
Fagron	Acetato de hidrocortisona	16J28-B05-330083	1
Fagron	Acetato de hidrocortisona	16J28-B51-333889	3
Fagron	Acetato de hidrocortisona	17086211	3
Fagron	Acetato de hidrocortisona	17219706	1
Fagron	Acetato de hidrocortisona	17C10	2
Fagron	Acetato de hidrocortisona	17C10-B01-333961	1
Fagron	Acetato de hidrocortisona	17C10-B01-333962	5
Fagron	Acetato de hidrocortisona	17C10-B01-335774	2
Fagron	Acetato de hidrocortisona	17G03	1
Fagron	Acetato de hidrocortisona	17G03-B06-338750	1
Fagron	Acetato de hidrocortisona	17G03-B06-341304	2
Fagron	Acetato de hidrocortisona	17g03-b06-341305	1
Fagron	Acetato de hidrocortisona	17G03-B06-341305	2
Fagron	Acetato de hidrocortisona	17G03-B06-341843	4
Fagron	Acetato de hidrocortisona	17G03-B06-345375	3
Fagron	Acetato de hidrocortisona	17GO3-B06-345375	1
Fagron	Acetato de hidrocortisona	17L19	2
Fagron	Acetato de hidrocortisona	17L19-B04	2
Fagron	Acetato de hidrocortisona	17L19B04345374	1
Fagron	Acetato de hidrocortisona	17L19-B04-345374	1
Fagron	Acetato de hidrocortisona	17L19-B04-348983	2
Fagron	Acetato de hidrocortisona	17L19-B04-350448	2
Fagron	Acetato de hidrocortisona	18142806	1
Fagron	Acetato de hidrocortisona	18278005	1
Fagron	Acetato de hidrocortisona	18H07	1
Fagron	Acetato de hidrocortisona	18H07-B03	3
Fagron	Acetato de hidrocortisona	18H07-B03-352228	8
Fagron	Acetato de hidrocortisona	18H07-B03-355044	2
Fagron	Acetato de hidrocortisona	18H07-B03-356259	4
Fagron	Acetato de hidrocortisona	18H07-B03-357240	7
Fagron	Acetato de hidrocortisona	18H07-BO3-357240	1
Fagron	Acetato de hidrocortisona	19090001	1
Fagron	Acetato de hidrocortisona	19A24B05	1
Fagron	Acetato de hidrocortisona	19A24-B05	3
Fagron	Acetato de hidrocortisona	19A24-B05-359123	1
Fagron	Acetato de hidrocortisona	19A24-B05359124	1
Fagron	Acetato de hidrocortisona	19A24-B05-359124	7
Fagron	Acetato de hidrocortisona	19A24-B05-361623	4
Fagron	Acetato de hidrocortisona	19A24-B05-361624	2
Fagron	Acetato de hidrocortisona	19A24-BO5-361623	1
Fagron	Acetato de hidrocortisona	19J00	1
Fagron	Acetato de hidrocortisona	19J10-f04	1
Fagron	Acetato de hidrocortisona	19J10-F04	2
Fagron	Acetato de hidrocortisona	19J10-F04-36627	1
Fagron	Acetato de hidrocortisona	19J10-F04366275	1
Fagron	Acetato de hidrocortisona	19J10-F04-366275	2
Fagron	Acetato de hidrocortisona	19J10-F04-366276	1
Fagron	Acetato de hidrocortisona	19j10-f04-366277	1
Fagron	Acetato de hidrocortisona	19J10-F04-366277	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Acetato de hidrocortisona	19j10-f04-366278	3
Fagron	Acetato de hidrocortisona	19MO-F04-366277	1
Fagron	Acetato de hidrocortisona	200508-1	1
Fagron	Acetato de hidrocortisona	20804-F07-370096	1
Fagron	Acetato de hidrocortisona	20B04-F07	1
Fagron	Acetato de hidrocortisona	20B04-F07-370094	2
Fagron	Acetato de hidrocortisona	20B04-F07-370095	1
Fagron	Acetato de hidrocortisona	20B04-F07-370096	1
Fagron	Acetato de hidrocortisona	20F19-F01-371737	1
Fagron	Acetato de hidrocortisona	20F19F01371738	1
Fagron	Acetato de hidrocortisona	20F19-F01-371740	3
Fagron	Acetato de hidrocortisona	20J13-F10	2
Fagron	Acetato de hidrocortisona	20J13-F10-375214	2
Fagron	Acetato de hidrocortisona	20J13-F10-375216	1
Fagron	Acetato de hidrocortisona	20J13-F10-375217	1
Fagron	Acetato de hidrocortisona	21d22-f01-378700	1
Fagron	Acetato de hidrocortisona	22A17-B07-216283	2
Fagron	Acetato de hidrocortisona	22A17-B07-216284	1
Fagron	Acetato de hidrocortisona	22A17-B07-216285	3
Fagron	Acetato de hidrocortisona	22H11-B01-220314	2
Fagron	Acetato de hidrocortisona	2OF19-F01-371737	1
Fagron	Acetato de hidrocortisona	32(20F19-F01-371738)	1
Fagron	Acetato de hidrocortisona	33(20F19-F01-371738)	1
Fagron	Acetato de hidrocortisona	345873/P-19091821	1
Fagron	Acetato de hidrocortisona	3613A-01718	1
Fagron	Acetato de hidrocortisona	7C10-B01-333961	1
Fagron	Acetato de hidrocortisona	8563642	1
Fagron	Acetato de hidrocortisona	B05-3591203	1
Fagron	Acetato de hidrocortisona	F01-3717308	2
Fagron	Acetato de hidrocortisona	F04-3662707	1
Fagron	Acetato de hidrocortisona	HC0024	1
Fagron	Acetato de hidrocortisona	M39171	1
Fagron	Acetato de hidrocortisona	NCEHAC130201	1
Fagron	Acetato de hidrocortisona	NCEHAC151101	1
Fagron	Acetato de hidrocortisona	NCEHAC170201	2
Fagron	Acetato de hidrocortisona	NCEHAC170507	4
Fagron	Acetato de hidrocortisona	NCEHAC181105	2
Fagron	Acetato de hidrocortisona	NCEHAC1900901	1
Fargon	Acetato de hidrocortisona	17L19-B04-345373	1
Fargon	Acetato de hidrocortisona	18H07-B03-356259	1
Fargon	Acetato de hidrocortisona	19A24-B05-361622	1
Fargon	Acetato de hidrocortisona	F01-3717308	1
Fargon	Acetato de hidrocortisona	F04-3662705	2
Faron/Noweda	Acetato de hidrocortisona	19A24_B05_361622	1
Fiebig	Acetato de hidrocortisona	1209003-01	1
Fiebig	Acetato de hidrocortisona	1605410	1
Fiebig	Acetato de hidrocortisona	16095404	2
Fiebig	Acetato de hidrocortisona	17219702	2
Fiebig	Acetato de hidrocortisona	17219703	1
Fiebig	Acetato de hidrocortisona	18142803	1
Fiebig	Acetato de hidrocortisona	18278006	1
Fiebig	Acetato de hidrocortisona	18278010	1
Finteler Apotheke	Acetato de hidrocortisona	1604052-01	2
Gatt-Koller	Acetato de hidrocortisona	1734/05154415	1
Gatt-Koller	Acetato de hidrocortisona	1802876	1
GEHE 03.07.2014	Acetato de hidrocortisona	14043903	1
Gehe amax	Acetato de hidrocortisona	16238712	1
Gehe amax	Acetato de hidrocortisona	18142807	2
Gehe amax	Acetato de hidrocortisona	18278008	2
Gehe amax	Acetato de hidrocortisona	18278019	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe Rostock	Acetato de hidrocortisona	20000978010	1
Gehe	Acetato de hidrocortisona	1205034-01	1
Gehe	Acetato de hidrocortisona	14043905	1
Gehe	Acetato de hidrocortisona	14144805	1
Gehe	Acetato de hidrocortisona	1501035-01	1
Gehe	Acetato de hidrocortisona	15356901	2
Gehe	Acetato de hidrocortisona	15356902	1
Gehe	Acetato de hidrocortisona	16004408	2
GEHE	Acetato de hidrocortisona	1604052-01	1
Gehe	Acetato de hidrocortisona	16095407	1
Gehe	Acetato de hidrocortisona	16238710	1
GEHE	Acetato de hidrocortisona	16238712	1
GEHE	Acetato de hidrocortisona	16238713	1
GEHE	Acetato de hidrocortisona	1706021-01	2
GEHE	Acetato de hidrocortisona	17219703	1
Gehe	Acetato de hidrocortisona	17219704	1
Gehe	Acetato de hidrocortisona	17219705	3
gehe	Acetato de hidrocortisona	17219707	1
Gehe	Acetato de hidrocortisona	17219707	3
Gehe	Acetato de hidrocortisona	1805010-01	4
Gehe	Acetato de hidrocortisona	18142804	1
Gehe	Acetato de hidrocortisona	18142812	2
Gehe	Acetato de hidrocortisona	18278004	2
Gehe	Acetato de hidrocortisona	18278010	1
gehe	Acetato de hidrocortisona	18278014	1
GEHE	Acetato de hidrocortisona	18278020	1
Gehe	Acetato de hidrocortisona	19138305	2
Gehe	Acetato de hidrocortisona	19138307	4
Gehe	Acetato de hidrocortisona	200004117001	1
Gehe	Acetato de hidrocortisona	20000978006	1
Gehe	Acetato de hidrocortisona	20000978009	1
Gehe	Acetato de hidrocortisona	21002415001	1
Gehe	Acetato de hidrocortisona	22002539008	2
Gehe	Acetato de hidrocortisona	22002539015	1
GEHE	Acetato de hidrocortisona	2205004-01	1
Gehe	Acetato de hidrocortisona	2306007-01	1
Geilenkirchen	Acetato de hidrocortisona	16238710	1
Geilenkirchen	Acetato de hidrocortisona	18142815	1
Geilenkirchen	Acetato de hidrocortisona	18278016	1
Geilenkirchen	Acetato de hidrocortisona	19138307	1
Geilenkirchen	Acetato de hidrocortisona	20000978004	1
Geilenkirchen	Acetato de hidrocortisona	20004117004	1
Hedinger/Gehe	Acetato de hidrocortisona	1112031-02	1
Hedinger/Sanacorp	Acetato de hidrocortisona	1706021-01	2
Henan Lihua Pharma. ...	Acetato de hidrocortisona	18142806	1
Henan Lihua Pharmace...	Acetato de hidrocortisona	20000978008	1
Henan Lihua Pharmace...	Acetato de hidrocortisona	2004029-01	1
Henan/Noweda	Acetato de hidrocortisona	K06M20190611	1
Henan/Noweda	Acetato de hidrocortisona	KD6M20190612	1
Henan/Phoenix	Acetato de hidrocortisona	K06M20190612	2
Henen / Gehe	Acetato de hidrocortisona	20000978004	1
Hepart	Acetato de hidrocortisona	14144804	1
Ichthyol GmbH/Noweda	Acetato de hidrocortisona	17086205	1
Jenne	Acetato de hidrocortisona	21002415006	1
Jenne	Acetato de hidrocortisona	23001089005	1
Kehr	Acetato de hidrocortisona	1706021-01	2
Kehr	Acetato de hidrocortisona	17L19-B04-347866	1
Kehr	Acetato de hidrocortisona	22002539008	1
Kehr	Acetato de hidrocortisona	22002539010	1
Kehr	Acetato de hidrocortisona	22002539013	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Acetato de hidrocortisona	22002539015	1
Kehr	Acetato de hidrocortisona	22H11-B01-224312	1
Kehr	Acetato de hidrocortisona	23001089005	2
Klenk	Acetato de hidrocortisona	1/06021-01	1
Klenk	Acetato de hidrocortisona	1112031-01	1
Klenk	Acetato de hidrocortisona	14301401	1
Klenk	Acetato de hidrocortisona	18142803	1
Krieger	Acetato de hidrocortisona	2205004-01	1
L10	Acetato de hidrocortisona	1706021-01	5
L12	Acetato de hidrocortisona	1604052-01	3
Lihua/phönix	Acetato de hidrocortisona	KO6A20140801M	1
Midas	Acetato de hidrocortisona	17219707	1
Nachprüfung	Acetato de hidrocortisona		1
Nachprüfung	Acetato de hidrocortisona	2082019-4	1
Noveda	Acetato de hidrocortisona	20000978008	1
Noweda /Cealo	Acetato de hidrocortisona	20000978004	1
Noweda 17.07.2015	Acetato de hidrocortisona	14301403	1
Noweda am 10.10.2017	Acetato de hidrocortisona	1706021	1
Noweda/ Pharmacia & ...	Acetato de hidrocortisona	1205034-01	1
Noweda/apotec	Acetato de hidrocortisona	2205004-01	1
Noweda/Euro	Acetato de hidrocortisona	1501035-01	1
Noweda	Acetato de hidrocortisona	1112031-02	1
Noweda	Acetato de hidrocortisona	13G09-N08	1
Noweda	Acetato de hidrocortisona	16095407	1
Noweda	Acetato de hidrocortisona	16095410	2
Noweda	Acetato de hidrocortisona	16238710	1
Noweda	Acetato de hidrocortisona	17219705	1
Noweda	Acetato de hidrocortisona	17219706	1
Noweda	Acetato de hidrocortisona	17219707	4
Noweda	Acetato de hidrocortisona	18142804	2
Noweda	Acetato de hidrocortisona	18142805	2
Noweda	Acetato de hidrocortisona	18142806	1
Noweda	Acetato de hidrocortisona	18142807	1
Noweda	Acetato de hidrocortisona	18142808	1
Noweda	Acetato de hidrocortisona	18278004	2
Noweda	Acetato de hidrocortisona	18278010	1
Noweda	Acetato de hidrocortisona	18278014	2
Noweda	Acetato de hidrocortisona	18278015	1
Noweda	Acetato de hidrocortisona	18278019	3
Noweda	Acetato de hidrocortisona	1907011-01	1
Noweda	Acetato de hidrocortisona	19138303	1
Noweda	Acetato de hidrocortisona	20000978005	1
Noweda	Acetato de hidrocortisona	20000978010	1
Noweda	Acetato de hidrocortisona	20004117005	2
Noweda	Acetato de hidrocortisona	20004117007	1
Noweda	Acetato de hidrocortisona	20004278004	1
Noweda	Acetato de hidrocortisona	21002415011	1
Noweda	Acetato de hidrocortisona	21002415014	1
Noweda	Acetato de hidrocortisona	2200253900	1
Noweda	Acetato de hidrocortisona	22002539001	1
Noweda	Acetato de hidrocortisona	22002539004	1
Noweda	Acetato de hidrocortisona	22002539005	3
Noweda	Acetato de hidrocortisona	22002539008	2
Noweda	Acetato de hidrocortisona	22002539012	2
Noweda	Acetato de hidrocortisona	22002539013	1
Noweda	Acetato de hidrocortisona	22002539014	1
Noweda	Acetato de hidrocortisona	22002539015	1
noweda	Acetato de hidrocortisona	2205004	1
Noweda	Acetato de hidrocortisona	2205004-01	1
Noweda	Acetato de hidrocortisona	23001089004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Acetato de hidrocortisona	caelo	1
Otto Fischer GmbH&Co...	Acetato de hidrocortisona	1907011-02	3
ph euro	Acetato de hidrocortisona	1907011-01	1
ph euro	Acetato de hidrocortisona	1907011-02	1
Pharmacia&Upjohn Com...	Acetato de hidrocortisona	1209003-01	1
Phoenix 14.01.2015 E...	Acetato de hidrocortisona	14043902	1
Phoenix 24.01.2019	Acetato de hidrocortisona	18278004	1
Phoenix Goettin	Acetato de hidrocortisona	1209003-01	1
Phoenix	Acetato de hidrocortisona	1209003-01	1
Phoenix	Acetato de hidrocortisona	12182402	1
Phoenix	Acetato de hidrocortisona	12330107	1
Phoenix	Acetato de hidrocortisona	1568/05131813	1
Phoenix	Acetato de hidrocortisona	15A30-B09	1
Phoenix	Acetato de hidrocortisona	15J28-B12	1
Phoenix	Acetato de hidrocortisona	16004403	1
Phoenix	Acetato de hidrocortisona	17086204	2
Phoenix	Acetato de hidrocortisona	17086205	1
Phoenix	Acetato de hidrocortisona	18142802	1
Phoenix	Acetato de hidrocortisona	18278015	1
Phoenix	Acetato de hidrocortisona	18278016	2
Phoenix	Acetato de hidrocortisona	18H07-B03-352227	1
Phoenix	Acetato de hidrocortisona	1907011-03	2
Phoenix	Acetato de hidrocortisona	19138304	1
Phoenix	Acetato de hidrocortisona	20000978004	1
Phoenix	Acetato de hidrocortisona	20004117001	1
Phoenix	Acetato de hidrocortisona	20004278004	1
Phoenix	Acetato de hidrocortisona	20004278008	1
Phoenix	Acetato de hidrocortisona	200303103	1
Phoenix	Acetato de hidrocortisona	2004029-01	2
Phoenix	Acetato de hidrocortisona	200421105	1
Phoenix	Acetato de hidrocortisona	22002539019	1
Phoenix	Acetato de hidrocortisona	23001089004	2
Phoenix	Acetato de hidrocortisona	3068	1
Phoenix	Acetato de hidrocortisona	3209	1
Phönix Gotha	Acetato de hidrocortisona	12182405	1
Phönix Gotha	Acetato de hidrocortisona	12330108	1
Phönix Gotha	Acetato de hidrocortisona	17219706	1
Phönix, Caesar&Loret...	Acetato de hidrocortisona	191383001	1
Phönix/Lihua	Acetato de hidrocortisona	1409005-01	1
Phönix	Acetato de hidrocortisona	1112031-01	1
Phönix	Acetato de hidrocortisona	1112031-02	1
Phönix	Acetato de hidrocortisona	1205034-01	1
Phönix	Acetato de hidrocortisona	12182405	1
Phönix	Acetato de hidrocortisona	12A13-N02	1
Phönix	Acetato de hidrocortisona	12K15-No4	1
Phönix	Acetato de hidrocortisona	14144804	2
phönix	Acetato de hidrocortisona	15356901	2
phönix	Acetato de hidrocortisona	16238708	1
phönix	Acetato de hidrocortisona	16238712	1
Phönix	Acetato de hidrocortisona	1706021-01	1
PHÖNIX	Acetato de hidrocortisona	17086211	1
Phönix	Acetato de hidrocortisona	17219705	1
Phönix	Acetato de hidrocortisona	1805010-01	1
Phönix	Acetato de hidrocortisona	18142802	1
phönix	Acetato de hidrocortisona	18142804	1
Phönix	Acetato de hidrocortisona	18142815	2
Phönix	Acetato de hidrocortisona	18278004	2
Phönix	Acetato de hidrocortisona	18278005	1
Phönix	Acetato de hidrocortisona	18278006	1
Phönix	Acetato de hidrocortisona	18278010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Acetato de hidrocortisona	18278014	1
Phönix	Acetato de hidrocortisona	18278016	1
Phönix	Acetato de hidrocortisona	19138302	3
PHÖNIX	Acetato de hidrocortisona	19138305	1
Phönix	Acetato de hidrocortisona	19138307	1
Phönix	Acetato de hidrocortisona	20000978004	1
Phönix	Acetato de hidrocortisona	20000978006	1
Phönix	Acetato de hidrocortisona	20000978010	1
phonix	Acetato de hidrocortisona	20004117001	1
Phönix	Acetato de hidrocortisona	20004278002	1
Phönix	Acetato de hidrocortisona	20004278003	1
PHÖNIX	Acetato de hidrocortisona	20004278003	1
Phönix	Acetato de hidrocortisona	20004278004	1
Phönix	Acetato de hidrocortisona	2000978007	1
Phönix	Acetato de hidrocortisona	2000978009	1
Phönix	Acetato de hidrocortisona	2004029-01	4
PHÖNIX	Acetato de hidrocortisona	21002415001	2
Phönix	Acetato de hidrocortisona	21002415002	1
Phönix	Acetato de hidrocortisona	21002415004	2
Phönix	Acetato de hidrocortisona	22002539014	1
Phönix	Acetato de hidrocortisona	22002539019	4
Phönix	Acetato de hidrocortisona	AKD8	1
Röntgen	Acetato de hidrocortisona	16095410	1
Röntgen	Acetato de hidrocortisona	17219705	1
Röntgen	Acetato de hidrocortisona	18278010	1
Röntgen	Acetato de hidrocortisona	19138307	1
Röntgen	Acetato de hidrocortisona	20000977002	1
Röntgen	Acetato de hidrocortisona	21002415010	1
Sanacorp	Acetato de hidrocortisona	1107004-03	1
Sanacorp	Acetato de hidrocortisona	11263913	1
Sanacorp	Acetato de hidrocortisona	12182404	2
Sanacorp	Acetato de hidrocortisona	12330103	1
Sanacorp	Acetato de hidrocortisona	13155302	2
Sanacorp	Acetato de hidrocortisona	13291704	1
Sanacorp	Acetato de hidrocortisona	14043903	1
Sanacorp	Acetato de hidrocortisona	1409005-01	3
sanacorp	Acetato de hidrocortisona	14301406	1
Sanacorp	Acetato de hidrocortisona	1501035-01	1
Sanacorp	Acetato de hidrocortisona	16095407	1
Sanacorp	Acetato de hidrocortisona	16238706	1
Sanacorp	Acetato de hidrocortisona	16238708	1
Sanacorp	Acetato de hidrocortisona	16238710	1
Sanacorp	Acetato de hidrocortisona	1706021-01	1
Sanacorp	Acetato de hidrocortisona	17219704	1
Sanacorp	Acetato de hidrocortisona	17219708	1
Sanacorp	Acetato de hidrocortisona	18142805	2
Sanacorp	Acetato de hidrocortisona	18278006	1
Sanacorp	Acetato de hidrocortisona	18278008	3
Sanacorp	Acetato de hidrocortisona	185010-01	1
Sanacorp	Acetato de hidrocortisona	191383004	1
Sanacorp	Acetato de hidrocortisona	20004117006	1
Sanacorp	Acetato de hidrocortisona	20004278003	6
Sanacorp	Acetato de hidrocortisona	20004278009	1
Sanacorp	Acetato de hidrocortisona	21002415001	1
Sanacorp	Acetato de hidrocortisona	22002539002	1
Sanacorp	Acetato de hidrocortisona	22002539008	1
Sanacorp	Acetato de hidrocortisona	22002539009	2
Sanacorp	Acetato de hidrocortisona	22002539010	1
Sanacorp	Acetato de hidrocortisona	23001089006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Acetato de hidrocortisona	2306007-01	3
SanacorpWE:13.02.201…	Acetato de hidrocortisona	1604052-01	1
sannacop	Acetato de hidrocortisona	2205004-01	1
Tianjin Jinjin Pharm…	Acetato de hidrocortisona	19138304	1
Tianjin Jinjin Pharm…	Acetato de hidrocortisona	18278019	1
Tianjin Jinjin/Gehe	Acetato de hidrocortisona	17L19-B04-345373	1
Tianjin/Noweda	Acetato de hidrocortisona	HD0027	1
Tianjin/Noweda	Acetato de hidrocortisona	HD0039	2
Wepa/Noweda	Acetato de hidrocortisona	20004117001	1
xxx	Acetato de hidrocortisona		1

- 230 479 spectra from 1515 *Apo-Ident* customers from a total of 48 671 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetato de hidrocortisona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetato de hidrocortisona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	429	0	152 533
Type B	0	1296	0	200 788
Type C	0	5548	40	230 479

The substance/substance group *Acetato de hidrocortisona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6014 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5370 %)
Type C	100.0000 % (> 99.9007 %)	99.2842 % (> 99.2305 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21295	21889	6,84	178,22
21462	21889	6,07	178,07
21889	21889	0,00	180,82
22241	21889	4,70	179,00
22564	22564	0,00	182,94
24392	24392	0,00	179,29
24590	22564	8,23	182,48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de noretisterona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20797-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de noretisterona; Norestisterona, acetato; Norethisteroni acetas

Special notes

When selecting the *Acetato de noretisterona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de noretisterona	7	3	48

Second-stage model

For differentiation of the substance/substance group *Acetato de noretisterona* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de noretisterona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	118,91	–
⋮	⋮	⋮
Prednicarbato	>50	99,79
Capsaicina	>50	101,88
Cloridrato de oxibutinina	>50	164,96
Alfaestradiol	>50	240,32
Citrato de sódio	>50	256,65
Tetracaína	>50	262,19
Levocarnitina	>50	268,30
Acetato de ciproterona	>50	323,42
Cloridrato de amitriptilina	>50	524,94
Piridoxal-5-fosfato	>50	548,62
Heparina sódica	>50	633,31
Valina	>50	655,40
Cloridrato de quinina di-hidratado	>50	718,33
Metoxisaleno	>50	789,25
Cloridrato de ciprofloxacina	>50	1079,05
Amifampridina	>50	2031,34
Sacarose	>50	2266,81
Triclosan	>50	2394,57

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de noretisterona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de noretisterona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetato de noretisterona	15417004	23122	40	1711489
Caelo	Acetato de noretisterona	182252	24395	40	20181031*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Acetato de noretisterona	1306033-01	21627	60	1511684
Euro OTC	Acetato de noretisterona	2401002	27151	40	20240321*
Euro OTC	Acetato de noretisterona	2401002	27151SI	30	20240321*
Fagron	Acetato de noretisterona	12L14-N03	20797	40	1401558
Fagron	Acetato de noretisterona	17B21-B01-341608	23918	40	20170619
Fagron	Acetato de noretisterona	19I30-F02-366139	25364	40	20191127
Fagron	Acetato de noretisterona	19I30-F02-366139	25364SI	20	20191127

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 350 spectra of 9 reference samples from the substance/substance group *Acetato de noretisterona*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 612 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Acetato de noretisterona*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Acetato de noretisterona	2106015	25771	40
Fagron	Acetato de noretisterona	14H29-B03-325225	23171	40
Fagron	Acetato de noretisterona	23H08-B10-227915	27025	40
Euro OTC	Acetato de noretisterona	2106015	25771SI	20
Fagron	Acetato de noretisterona	23H08-B10-227915	27025SI	30

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 914 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 63 spectra from 36 *Apo-Ident* customers from 53 batches from the substance/substance group *Acetato de noretisterona*.

- Among them are spectra of independent samples from 47 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bombastus	Acetato de noretisterona	13J08-N04	1
Caelo	Acetato de noretisterona	15417001	1
Caelo	Acetato de noretisterona	15417008	1
Caelo	Acetato de noretisterona	16081814	1
Caelo	Acetato de noretisterona	17B21-B01-335383	1
Euro OTC	Acetato de noretisterona	1306033-02	2
Euro/Phönix	Acetato de noretisterona	1306033-01	1
Fagron	Acetato de noretisterona		1
Fagron	Acetato de noretisterona	12C06-N10	2
Fagron	Acetato de noretisterona	13D19-N06	1
Fagron	Acetato de noretisterona	13J08-N04	1
Fagron	Acetato de noretisterona	14d08-b01-292736	1
Fagron	Acetato de noretisterona	14D08-B01-292738	1
Fagron	Acetato de noretisterona	14H29-B03	1
Fagron	Acetato de noretisterona	14H29-B03-299313	1
Fagron	Acetato de noretisterona	14H29-B03-302277	2
Fagron	Acetato de noretisterona	14h29-b03-310697	1
Fagron	Acetato de noretisterona	14H29-B03-321322	1
Fagron	Acetato de noretisterona	14H29-B03-325224	1
Fagron	Acetato de noretisterona	17B21-B01	1
Fagron	Acetato de noretisterona	17B21-B01-335384	1
Fagron	Acetato de noretisterona	17B21-B01-341607	2
Fagron	Acetato de noretisterona	17B21-B01-341608	1
Fagron	Acetato de noretisterona	17B21-B01-344250	1
Fagron	Acetato de noretisterona	18C12-B03-347998	1
Fagron	Acetato de noretisterona	18C12-B03-349111	1
Fagron	Acetato de noretisterona	18C12-B03-349157	2
Fagron	Acetato de noretisterona	18C12-B03-353056	1
Fagron	Acetato de noretisterona	18C12-B03-354813	1
Fagron	Acetato de noretisterona	18C12-B03-354815	2
Fagron	Acetato de noretisterona	18L14-B05	2
Fagron	Acetato de noretisterona	18L14-B05-358972	1
Fagron	Acetato de noretisterona	18L14-B05-358976	1
Fagron	Acetato de noretisterona	18L14-B05-358977	1
Fagron	Acetato de noretisterona	19/30-F02-366134	1
Fagron	Acetato de noretisterona	19130-F02-373337	1
Fagron	Acetato de noretisterona	19I30-F02-366134	1
Fagron	Acetato de noretisterona	19I30-f02-366139	1
Fagron	Acetato de noretisterona	19I30-F02-366139	1
Fagron	Acetato de noretisterona	19I30-F02-3688303	1
Fagron	Acetato de noretisterona	21g12-b02-213688	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Acetato de noretisterona	21G12-B02-213688	1
Fagron	Acetato de noretisterona	21G12-B02-213691	2
Fagron	Acetato de noretisterona	21G12-B02	1
Fagron	Acetato de noretisterona	22061206	1
Fagron	Acetato de noretisterona	23071509	1
Fagron	Acetato de noretisterona	F02-3661309	1
Fagron	Acetato de noretisterona	F02-3733307	2
Gehe	Acetato de noretisterona	14H29-B03-321324	1
Gehe	Acetato de noretisterona	15417011	1
GEHE	Acetato de noretisterona	18L-14B05	1
Phoenix	Acetato de noretisterona	17B21B01335384	1
Phönix	Acetato de noretisterona	14H29-B03-315702	1
Phönix	Acetato de noretisterona	F02-3661305	1

- 236 004 spectra from 1515 *Apo-Ident* customers from a total of 49 205 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetato de noretisterona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetato de noretisterona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	350	0	152 612
Type B	0	170	0	201 914
Type C	0	61	2	236 004

The substance/substance group *Acetato de noretisterona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2857 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	96.8254 % (> 92.0635 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20797	20797	0,00	147,33
21627	21627	0,00	141,48
23122	23122	0,00	144,30
23918	24395	3,91	147,63
24395	24395	0,00	147,96
25364	24395	4,52	148,28
27151	27151	0,00	138,05

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de prednisolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20089-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de prednisolona; Prednisolona, acetato; Prednisoloni acetas

Special notes

When selecting the *Acetato de prednisolona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de prednisolona	9	13	420

Second-stage model

For differentiation of the substance/substance group *Acetato de prednisolona* the following second-stage model is used:

- Submodelo 08

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de prednisolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisona	73,25	50,42
⋮	⋮	⋮
Cloridrato de efedrina	>50	146,64

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de prednisolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de prednisolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetato de prednisolona	12091814	20784	80	20120416
Caelo	Acetato de prednisolona	12324502	20877	40	20121112
Caelo	Acetato de prednisolona	13262605	21448	60	20130923
Caelo	Acetato de prednisolona	13262605	21450	60	20130923
Caelo	Acetato de prednisolona	13262605	21450SI	47	20130923
Euro OTC	Acetato de prednisolona	1306040	21096	40	20130812
Euro OTC	Acetato de prednisolona	1209028-03	21530	60	AR-15-FG-010480-01
Euro OTC	Acetato de prednisolona	1512020	22297	45	20160119*
Euro OTC	Acetato de prednisolona	1512020	22297SI	44	20160119*
Euro OTC	Acetato de prednisolona	2010016	25525	40	20210104*
Euro OTC	Acetato de prednisolona	2010016	25525SI	40	20210104*
Fagron	Acetato de prednisolona	12H14-N07	20795	40	20120829
Fagron	Acetato de prednisolona	12H14-N07	20795SI	49	20120829
Fagron	Acetato de prednisolona	15I23-B04-345785	24587	40	20151014

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 685 spectra of 14 reference samples from the substance/substance group *Acetato de prednisolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 277 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1098 spectra of 28 reference samples from the substance/substance group *Acetato de prednisolona*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetato de prednisolona	180673	24534	40
Caelo	Acetato de prednisolona	20001950	25215	40
Caelo	Acetato de prednisolona	22001230	26129	30
Euro OTC	Acetato de prednisolona	1607010	22710	40
Euro OTC	Acetato de prednisolona	1701041	23142	40
Euro OTC	Acetato de prednisolona	1805009	24133	40
Euro OTC	Acetato de prednisolona	1903031	24636	40
Euro OTC	Acetato de prednisolona	1911014	24960	40
Euro OTC	Acetato de prednisolona	2201028	25954	40
Euro OTC	Acetato de prednisolona	2309013	27008	30
Euro OTC	Acetato de prednisolona	2410006	27459	30
Fagron	Acetato de prednisolona	21K18-B05-220957	26169	40
Fagron	Acetato de prednisolona	23G05-B13-228543	26916	40
Caelo	Acetato de prednisolona	13262605	21448SI†	44
Caelo	Acetato de prednisolona	180673	24534SI	80
Caelo	Acetato de prednisolona	20001950	25215SI	40
Caelo	Acetato de prednisolona	22001230	26129SI	40
Euro OTC	Acetato de prednisolona	1607010	22710SI	40
Euro OTC	Acetato de prednisolona	1701041	23142SI	24
Euro OTC	Acetato de prednisolona	1805009	24133SI	40

continued on the next page

descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Acetato de prednisolona	1903031	24636SI	40
Euro OTC	Acetato de prednisolona	1911014	24960SI	40
Euro OTC	Acetato de prednisolona	2201028	25954SI	40
Euro OTC	Acetato de prednisolona	2309013	27008SI	40
Euro OTC	Acetato de prednisolona	2410006	27459SI	30
Fagron	Acetato de prednisolona	15I23-B04-345785	24587SI[†]	40
Fagron	Acetato de prednisolona	21K18-B05-220957	26169SI	30
Fagron	Acetato de prednisolona	23G05-B13-228543	26916SI	40

- 200 986 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3573 spectra from 1047 *Apo-Ident* customers from 435 batches from the substance/substance group *Acetato de prednisolona*.

- Among them are spectra of independent samples from 419 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Acetato de prednisolona	15398303	1
	Acetato de prednisolona	17086101	1
	Acetato de prednisolona	21001844007	1
	Acetato de prednisolona	21001844008	2
	Acetato de prednisolona	21001844012	7
	Acetato de prednisolona	22001230001	5
	Acetato de prednisolona	22001230002	3
	Acetato de prednisolona	22001230003	6
	Acetato de prednisolona	22001230004	5
	Acetato de prednisolona	22001230005	9
	Acetato de prednisolona	22001230007	9
	Acetato de prednisolona	22001230008	2
	Acetato de prednisolona	22001230009	2
	Acetato de prednisolona	2201028	2
	Acetato de prednisolona	2201028-01	10
	Acetato de prednisolona	2201028-02	11
	Acetato de prednisolona	22I27-B10-223685	1
	Acetato de prednisolona	230901301	1
	Acetato de prednisolona	2309013-01	10
	Acetato de prednisolona	B10-2236805	1
	Acetato de prednisolona	B10-2237606	1
A.H. 23.05.13 ek: 5,40EUR	Acetato de prednisolona	13A07-N07	1
A.H.D.	Acetato de prednisolona	14175514	1
AHD 06.03.15	Acetato de prednisolona	14175508	1
AHD 23.10.14 EK17,24	Acetato de prednisolona	13262601	1
AHD/Euro	Acetato de prednisolona	1805009-001	1
AHD	Acetato de prednisolona	15055202	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Acetato de prednisolona	17086105	1
AHD	Acetato de prednisolona	1903031-01	1
AHD	Acetato de prednisolona	22001230001	1
AHD	Acetato de prednisolona	22001230002	1
AHD	Acetato de prednisolona	22001230003	3
AHD	Acetato de prednisolona	22001230004	1
AHD	Acetato de prednisolona	22001230007	1
Alliamce Healthcare	Acetato de prednisolona	22001230001	1
Alliance Healthcare	Acetato de prednisolona	12091807	1
Alliance Healthcare	Acetato de prednisolona	1903031-02	1
Alliance Healthcare	Acetato de prednisolona	1911014-02	2
Alliance Healthcare	Acetato de prednisolona	20001950001	1
Alliance Healthcare	Acetato de prednisolona	2010016-01	7
Alliance Healthcare	Acetato de prednisolona	22001230007	1
Alliance Healthcare	Acetato de prednisolona	2309013-01	4
Alliance	Acetato de prednisolona	1209028-02	2
Alliance	Acetato de prednisolona	22001230004	1
Alliance	Acetato de prednisolona	K07A20190507	1
AllianceHealthcare	Acetato de prednisolona	15055201	1
Allianz Healthcare	Acetato de prednisolona	18067310	1
Anuh Pharma	Acetato de prednisolona	21001844006	1
ANZAG	Acetato de prednisolona	12091802	2
Anzag	Acetato de prednisolona	13A07N07	1
Anzag	Acetato de prednisolona	16246812	1
Anzag	Acetato de prednisolona	192969005	1
apo-ident/Noweda	Acetato de prednisolona	2010016-01	1
apo-ident/Phoenix	Acetato de prednisolona	190272002	1
apo-ident	Acetato de prednisolona	1512020-01	1
apo-ident	Acetato de prednisolona	1805009-02	1
apomix	Acetato de prednisolona	16246804	1
Avik Pharmaceutical ...	Acetato de prednisolona	19C28-B02-361964	1
Beiersdorf AG	Acetato de prednisolona	15055201	1
Beiersdorf AG	Acetato de prednisolona	15398302	1
Bombastus	Acetato de prednisolona	17185601	1
Bombastus	Acetato de prednisolona	2255	1
cae	Acetato de prednisolona	21001844004	1
Caeasar/Loretz,Fa.Gehe	Acetato de prednisolona	14380910	1
Cael Sanacorp 05.02.2016	Acetato de prednisolona	14175509	1
Cael Sanacorp 05.02.2016	Acetato de prednisolona	14380901	1
Caeleo/ Kehr	Acetato de prednisolona	21001844002	1
Caelo	Acetato de prednisolona		5
Caelo	Acetato de prednisolona	11080403	1
Caelo	Acetato de prednisolona	11158002	1
Caelo	Acetato de prednisolona	11158003	1
Caelo	Acetato de prednisolona	11L21-N03	1
Caelo	Acetato de prednisolona	12001844003	1
Caelo	Acetato de prednisolona	1209028-02	2
Caelo	Acetato de prednisolona	12091802	6
Caelo	Acetato de prednisolona	12091803	3
Caelo	Acetato de prednisolona	12091804	8
Caelo	Acetato de prednisolona	12091806	3
Caelo	Acetato de prednisolona	12091807	5
Caelo	Acetato de prednisolona	12091808	5
Caelo	Acetato de prednisolona	12091810	2
Caelo	Acetato de prednisolona	12091813	1
Caelo	Acetato de prednisolona	12091814	7
Caelo	Acetato de prednisolona	12091815	2
Caelo	Acetato de prednisolona	12324502	13
Caelo	Acetato de prednisolona	12324503	1
Caelo	Acetato de prednisolona	12324504	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de prednisolona	12324505	16
Caelo	Acetato de prednisolona	12324506	11
Caelo	Acetato de prednisolona	12324508	9
Caelo	Acetato de prednisolona	12324509	2
Caelo	Acetato de prednisolona	12324514	5
Caelo	Acetato de prednisolona	1234506	1
Caelo	Acetato de prednisolona	12L05-N01	1
Caelo	Acetato de prednisolona	1306040-01	1
Caelo	Acetato de prednisolona	1306040-02	1
Caelo	Acetato de prednisolona	13121715	1
Caelo	Acetato de prednisolona	13262601	17
Caelo	Acetato de prednisolona	13262602	8
Caelo	Acetato de prednisolona	13262603	8
Caelo	Acetato de prednisolona	13262605	13
Caelo	Acetato de prednisolona	13262606	4
Caelo	Acetato de prednisolona	13262609	4
Caelo	Acetato de prednisolona	13343112	1
Caelo	Acetato de prednisolona	1406014-01	2
Caelo	Acetato de prednisolona	1406014-02	2
Caelo	Acetato de prednisolona	14175508	16
Caelo	Acetato de prednisolona	14175509	9
Caelo	Acetato de prednisolona	14175512	1
Caelo	Acetato de prednisolona	14175513	10
Caelo	Acetato de prednisolona	14175514	7
Caelo	Acetato de prednisolona	14380302	1
Caelo	Acetato de prednisolona	14380901	19
Caelo	Acetato de prednisolona	14380902	14
Caelo	Acetato de prednisolona	14380903	2
Caelo	Acetato de prednisolona	14380904	2
Caelo	Acetato de prednisolona	14380905	21
Caelo	Acetato de prednisolona	14380909	14
Caelo	Acetato de prednisolona	14380910	10
Caelo	Acetato de prednisolona	1475509	1
Caelo	Acetato de prednisolona	1480905	1
Caelo	Acetato de prednisolona	15055201	9
Caelo	Acetato de prednisolona	15055202	16
Caelo	Acetato de prednisolona	15055203	2
Caelo	Acetato de prednisolona	15055206	10
Caelo	Acetato de prednisolona	151202001	1
Caelo	Acetato de prednisolona	1512020-01	4
Caelo	Acetato de prednisolona	1523-B04-336299	1
Caelo	Acetato de prednisolona	15298401	1
Caelo	Acetato de prednisolona	15344002	1
Caelo	Acetato de prednisolona	15396304	1
Caelo	Acetato de prednisolona	15398302	14
Caelo	Acetato de prednisolona	15398303	10
Caelo	Acetato de prednisolona	15398304	8
Caelo	Acetato de prednisolona	15398306	6
Caelo	Acetato de prednisolona	15398307	10
Caelo	Acetato de prednisolona	15398401	12
Caelo	Acetato de prednisolona	15398402	15
Caelo	Acetato de prednisolona	15398407	10
Caelo	Acetato de prednisolona	15398408	11
Caelo	Acetato de prednisolona	15B03B05302564	1
Caelo	Acetato de prednisolona	15B03-B05-302564	2
Caelo	Acetato de prednisolona	16/AKD2	1
Caelo	Acetato de prednisolona	160701001	3
Caelo	Acetato de prednisolona	1607010-01	6
Caelo	Acetato de prednisolona	1616I-02106	1
Caelo	Acetato de prednisolona	162446808	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de prednisolona	162468	2
Caelo	Acetato de prednisolona	16246801	19
Caelo	Acetato de prednisolona	16246802	12
Caelo	Acetato de prednisolona	16246803	20
Caelo	Acetato de prednisolona	16246803-14317/1	1
Caelo	Acetato de prednisolona	16246803-70317/1	1
Caelo	Acetato de prednisolona	16246804	14
Caelo	Acetato de prednisolona	16246805	2
Caelo	Acetato de prednisolona	16246806	15
Caelo	Acetato de prednisolona	16246807	18
Caelo	Acetato de prednisolona	16246808	15
Caelo	Acetato de prednisolona	16246809	3
Caelo	Acetato de prednisolona	16246811	8
Caelo	Acetato de prednisolona	16246812	11
Caelo	Acetato de prednisolona	1624801	1
Caelo	Acetato de prednisolona	1624806	1
Caelo	Acetato de prednisolona	16248808	1
Caelo	Acetato de prednisolona	165246802	1
Caelo	Acetato de prednisolona	170104-01	1
Caelo	Acetato de prednisolona	170104101	2
Caelo	Acetato de prednisolona	1701041-01	5
Caelo	Acetato de prednisolona	1701041-02	4
Caelo	Acetato de prednisolona	17041802	1
Caelo	Acetato de prednisolona	17086101	25
Caelo	Acetato de prednisolona	170861015494	1
Caelo	Acetato de prednisolona	17086102	12
Caelo	Acetato de prednisolona	17086103	19
Caelo	Acetato de prednisolona	17086103/1110917	1
Caelo	Acetato de prednisolona	17086104	26
Caelo	Acetato de prednisolona	17086105	26
Caelo	Acetato de prednisolona	17086106	2
Caelo	Acetato de prednisolona	17185601	30
Caelo	Acetato de prednisolona	171856010	1
Caelo	Acetato de prednisolona	17185602	29
Caelo	Acetato de prednisolona	17185603	30
Caelo	Acetato de prednisolona	17185604	4
Caelo	Acetato de prednisolona	17401041-02	1
Caelo	Acetato de prednisolona	1786103	1
Caelo	Acetato de prednisolona	18004401	28
Caelo	Acetato de prednisolona	18004402	22
Caelo	Acetato de prednisolona	18004403	3
Caelo	Acetato de prednisolona	18004903	1
Caelo	Acetato de prednisolona	1805009	1
Caelo	Acetato de prednisolona	180500901	1
Caelo	Acetato de prednisolona	1805009-01	6
Caelo	Acetato de prednisolona	1805009-02	2
Caelo	Acetato de prednisolona	180500903	1
Caelo	Acetato de prednisolona	1805009-03	1
Caelo	Acetato de prednisolona	18067301	4
Caelo	Acetato de prednisolona	18067302	24
Caelo	Acetato de prednisolona	180673025724	1
Caelo	Acetato de prednisolona	18067303	28
Caelo	Acetato de prednisolona	18067307	38
Caelo	Acetato de prednisolona	18067308	3
Caelo	Acetato de prednisolona	18067309	36
Caelo	Acetato de prednisolona	18067309P-190226-2	1
Caelo	Acetato de prednisolona	18067309-P20180115Ma	1
Caelo	Acetato de prednisolona	18067310	30
Caelo	Acetato de prednisolona	18067313	1
Caelo	Acetato de prednisolona	18067314	30

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de prednisolona	18067314P-191022-8	1
Caelo	Acetato de prednisolona	18067316	1
Caelo	Acetato de prednisolona	18067317	21
Caelo	Acetato de prednisolona	18067320	48
Caelo	Acetato de prednisolona	18067323	2
Caelo	Acetato de prednisolona	18067324	28
Caelo	Acetato de prednisolona	18067324-B04	1
Caelo	Acetato de prednisolona	18067325	6
Caelo	Acetato de prednisolona	18398303	1
Caelo	Acetato de prednisolona	1867309	1
Caelo	Acetato de prednisolona	1867314	1
Caelo	Acetato de prednisolona	19010303	1
Caelo	Acetato de prednisolona	1903031-01	3
Caelo	Acetato de prednisolona	1911014-01	1
Caelo	Acetato de prednisolona	1911014-02	3
Caelo	Acetato de prednisolona	19269004	2
Caelo	Acetato de prednisolona	192969003	33
Caelo	Acetato de prednisolona	192969004	35
Caelo	Acetato de prednisolona	192969004P-200220-2	1
Caelo	Acetato de prednisolona	192969005	38
Caelo	Acetato de prednisolona	19J08-F02-365546	1
Caelo	Acetato de prednisolona	19J0B-F02-366051	1
Caelo	Acetato de prednisolona	2000019500002	1
Caelo	Acetato de prednisolona	20001950001	12
Caelo	Acetato de prednisolona	200019500010	1
Caelo	Acetato de prednisolona	20001950002	18
Caelo	Acetato de prednisolona	20001950003	12
Caelo	Acetato de prednisolona	20001950004	13
Caelo	Acetato de prednisolona	2000195001	1
Caelo	Acetato de prednisolona	2000195004	1
Caelo	Acetato de prednisolona	200019550002	1
Caelo	Acetato de prednisolona	200034843003	1
Caelo	Acetato de prednisolona	20003817016	1
Caelo	Acetato de prednisolona	20003843001	32
Caelo	Acetato de prednisolona	20003843003	43
Caelo	Acetato de prednisolona	2000384300301972024	1
Caelo	Acetato de prednisolona	20003843004	21
Caelo	Acetato de prednisolona	200038443001	1
Caelo	Acetato de prednisolona	200038443003	1
Caelo	Acetato de prednisolona	20160727Ma1	1
Caelo	Acetato de prednisolona	21001844001	1
Caelo	Acetato de prednisolona	21001844002	23
Caelo	Acetato de prednisolona	21001844003	22
Caelo	Acetato de prednisolona	21001844004	15
Caelo	Acetato de prednisolona	21001844006	12
Caelo	Acetato de prednisolona	21001844006/221228	1
Caelo	Acetato de prednisolona	21001844007	18
Caelo	Acetato de prednisolona	21001844008	10
Caelo	Acetato de prednisolona	21001844010	5
Caelo	Acetato de prednisolona	21001844012	1
Caelo	Acetato de prednisolona	21001844013	1
Caelo	Acetato de prednisolona	2100184402	1
Caelo	Acetato de prednisolona	2100184404	1
Caelo	Acetato de prednisolona	2101844002	1
Caelo	Acetato de prednisolona	21071808	1
Caelo	Acetato de prednisolona	22001230001	7
Caelo	Acetato de prednisolona	22001230002	7
Caelo	Acetato de prednisolona	22001230003	6
Caelo	Acetato de prednisolona	22001230004	1
Caelo	Acetato de prednisolona	2200123001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de prednisolona	2200123002	1
Caelo	Acetato de prednisolona	23051812	1
Caelo	Acetato de prednisolona	26011905	1
Caelo	Acetato de prednisolona	27051301	1
Caelo	Acetato de prednisolona	313I-02106	1
Caelo	Acetato de prednisolona	32304	1
Caelo	Acetato de prednisolona	32304015	1
Caelo	Acetato de prednisolona	4313A-02106	1
Caelo	Acetato de prednisolona	5031511	1
Caelo	Acetato de prednisolona	5398304	1
Caelo	Acetato de prednisolona	6021306	1
Caelo	Acetato de prednisolona	717Q-02106	1
Caelo	Acetato de prednisolona	8067320	1
Caelo	Acetato de prednisolona	80673201	1
Caelo	Acetato de prednisolona	8699	1
Caelo	Acetato de prednisolona	F02-3660501	1
Caeol/Noweda	Acetato de prednisolona	16246802	1
Caesar & Lorenz GmbH	Acetato de prednisolona	21001844006	1
Caesar & Loretz GmbH...	Acetato de prednisolona	18067310	1
Caesar & Loretz GmbH...	Acetato de prednisolona	17185603	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20001950003	1
Caesar & Loretz GmbH...	Acetato de prednisolona	21001844008	1
Caesar & Loretz GmbH...	Acetato de prednisolona	192969003	1
Caesar & Loretz GmbH...	Acetato de prednisolona	192969003	1
Caesar & Loretz GmbH...	Acetato de prednisolona	17086105	1
Caesar & Loretz GmbH...	Acetato de prednisolona	17185601	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20003843003	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20001950001	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20003843004	3
Caesar & Loretz GmbH...	Acetato de prednisolona	21000607004	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20003843001	1
Caesar & Loretz GmbH/E	Acetato de prednisolona	192969005	1
Caesar & Loretz GmbH...	Acetato de prednisolona	18067320	1
Caesar & Loretz GmbH...	Acetato de prednisolona	192969005	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20003843003	1
Caesar & Loretz GmbH/Gehe	Acetato de prednisolona	18067324	1
Caesar & Loretz GmbH/Gehe	Acetato de prednisolona	192969003	1
Caesar & Loretz GmbH/Gehe	Acetato de prednisolona	21001844002	1
Caesar & Loretz GmbH/Gehe	Acetato de prednisolona	21001844007	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20001950004	2
Caesar & Loretz GmbH...	Acetato de prednisolona	22001230001	1
Caesar & Loretz GmbH...	Acetato de prednisolona	18067320	1
Caesar & Loretz GmbH...	Acetato de prednisolona	192969004	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20003843001	1
Caesar & Loretz GmbH/Kehr	Acetato de prednisolona	192969004	1
Caesar & Loretz GmbH...	Acetato de prednisolona	18067320	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20C06-F02-3700407	1
Caesar & Loretz GmbH...	Acetato de prednisolona	F12-3742909	1
Caesar & Loretz GmbH/Ph	Acetato de prednisolona	192969005	1
Caesar & Loretz GmbH...	Acetato de prednisolona	22001230001	3
Caesar & Loretz GmbH...	Acetato de prednisolona	1911014-02	1
Caesar & Loretz GmbH...	Acetato de prednisolona	192969005	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20001950004	1
Caesar & Loretz GmbH...	Acetato de prednisolona	20003843003	1
Caesar & Loretz GmbH...	Acetato de prednisolona	21001844003	2
Caesar & Loretz GmbH...	Acetato de prednisolona	21001844008	1
Caesar & Loretz GmbH...	Acetato de prednisolona	22001230001	1
Caesar & Loretz GmbH...	Acetato de prednisolona	22001230004	1
Caesar & Loretz GmbH...	Acetato de prednisolona	22001230002	1
Caesar & Loretz GmbH	Acetato de prednisolona	17185603	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Acetato de prednisolona	180667317	1
Caesar & Loretz GmbH	Acetato de prednisolona	18067303	1
Caesar & Loretz GmbH	Acetato de prednisolona	18067307	5
Caesar & Loretz GmbH	Acetato de prednisolona	18067309	2
Caesar & Loretz GmbH	Acetato de prednisolona	18067310	10
Caesar & Loretz GmbH	Acetato de prednisolona	18067314	7
Caesar & Loretz GmbH	Acetato de prednisolona	18067317	9
Caesar & Loretz GmbH	Acetato de prednisolona	18067320	3
Caesar & Loretz GmbH	Acetato de prednisolona	18067323	1
Caesar & Loretz GmbH	Acetato de prednisolona	18067324	1
Caesar & Loretz GmbH	Acetato de prednisolona	18067325	1
Caesar & Loretz GmbH	Acetato de prednisolona	1903031-01	1
Caesar & Loretz GmbH	Acetato de prednisolona	192969002	1
Caesar & Loretz GmbH	Acetato de prednisolona	192969003	5
Caesar & Loretz GmbH	Acetato de prednisolona	192969004	8
Caesar & Loretz GmbH	Acetato de prednisolona	192969005	15
Caesar & Loretz GmbH	Acetato de prednisolona	20001950001	11
Caesar & Loretz GmbH	Acetato de prednisolona	20001950002	9
Caesar & Loretz GmbH	Acetato de prednisolona	20001950003	9
Caesar & Loretz GmbH	Acetato de prednisolona	20001950004	8
Caesar & Loretz GmbH	Acetato de prednisolona	20001950005	3
Caesar & Loretz GmbH	Acetato de prednisolona	20003843001	11
Caesar & Loretz GmbH	Acetato de prednisolona	20003843002	1
Caesar & Loretz GmbH	Acetato de prednisolona	20003843003	13
Caesar & Loretz GmbH	Acetato de prednisolona	20003843004	9
Caesar & Loretz GmbH	Acetato de prednisolona	2001950002	1
Caesar & Loretz GmbH	Acetato de prednisolona	21001844002	6
Caesar & Loretz GmbH	Acetato de prednisolona	21001844003	10
Caesar & Loretz GmbH	Acetato de prednisolona	21001844004	9
Caesar & Loretz GmbH	Acetato de prednisolona	21001844006	4
Caesar & Loretz GmbH	Acetato de prednisolona	21001844007	1
Caesar & Loretz GmbH	Acetato de prednisolona	21001844008	5
Caesar & Loretz GmbH	Acetato de prednisolona	21001844010	2
Caesar & Loretz GmbH	Acetato de prednisolona	22001230001	3
Caesar & Loretz GmbH	Acetato de prednisolona	22001230003	1
Caesar & Loretz GmbH	Acetato de prednisolona	22001230004	1
Caesar & Loretz Hild…	Acetato de prednisolona	18067317	1
Caesar & Loretz/Geil…	Acetato de prednisolona	18067320	1
Caesar / Ebert & Jacobi	Acetato de prednisolona	17185603	1
Caesar Loretz	Acetato de prednisolona	192969005	2
Caesar&Loretz GmbH,P…	Acetato de prednisolona	17086103	2
Caesar&Loretz GmbH	Acetato de prednisolona	15396408	1
Caesar&Loretz GmbH	Acetato de prednisolona	18067324	1
Caesar&Loretz GmbH	Acetato de prednisolona	20003843003	1
Caesar&Loretz GmbH	Acetato de prednisolona	22001230002	1
Caesar&loretz,AHC,29…	Acetato de prednisolona	15398306	1
Caesar&loretz,Phoeni…	Acetato de prednisolona		1
Caesar&loretz,Phoenix	Acetato de prednisolona	13262606	1
Caesar&loretz,Phoenix	Acetato de prednisolona	14175513	1
Caesar&Loretz,Phönix…	Acetato de prednisolona	15398302	1
caesar&loretz,Phönix	Acetato de prednisolona	15055202	2
caesar&loretz	Acetato de prednisolona	14380909	1
Caesar&Loretz	Acetato de prednisolona	18067320	1
Caesar&LoretzGmbH,11…	Acetato de prednisolona	16246803	1
Cealo/Gehe	Acetato de prednisolona	20001950002	1
Cealo	Acetato de prednisolona	14175513	1
cealo	Acetato de prednisolona	18067303	1
Cealo	Acetato de prednisolona	19296004	1
Cealo	Acetato de prednisolona	192969005	1
Cealo	Acetato de prednisolona	20001950001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo	Acetato de prednisolona	21001844004	1
Ceasar & Loretz GmbH...	Acetato de prednisolona	18067303	1
Delta	Acetato de prednisolona	17086103	1
Delta	Acetato de prednisolona	17185602	1
Delta	Acetato de prednisolona	18067314	1
Ebert & Jacobi	Acetato de prednisolona	15398307	1
EuRho / Fiebig	Acetato de prednisolona	1903031-01	1
EuRho / Gehe	Acetato de prednisolona	1903031-01	1
EuRho/Gehe	Acetato de prednisolona	1805009-03	1
EuRho/Noweda	Acetato de prednisolona	18004401	1
EuRho/Phönix	Acetato de prednisolona	1805009-03	1
EuRho/Phönix	Acetato de prednisolona	1903031-01	1
Eurho/Phönix	Acetato de prednisolona	201001601	1
EuRho/Phönix	Acetato de prednisolona	201001601	1
EuRho/Phönix	Acetato de prednisolona	2010016-01	1
Eurho/Sanacorp	Acetato de prednisolona	1805009-01	2
EuRho/Sanacorp	Acetato de prednisolona	1903031-01	3
EuRho/Sanacorp	Acetato de prednisolona	1911014-01	2
EuRho	Acetato de prednisolona	1306040-03	1
EuRho	Acetato de prednisolona	1406014-02	1
EuRho	Acetato de prednisolona	1512020-01	1
Eurho	Acetato de prednisolona	1701041-01	2
EuRho	Acetato de prednisolona	1701041-01	1
EuRho	Acetato de prednisolona	170104102	1
EuRho	Acetato de prednisolona	1701041-02	1
EuRho	Acetato de prednisolona	1805009-01	2
EuRho	Acetato de prednisolona	1805009-02	1
EuRho	Acetato de prednisolona	1911014-01	3
EuRho	Acetato de prednisolona	1911014-02	1
EuRho	Acetato de prednisolona	2010016-01	3
Euro OTC	Acetato de prednisolona		1
Euro OTC	Acetato de prednisolona	1/01041-01	1
Euro OTC	Acetato de prednisolona	1108043-01	2
Euro OTC	Acetato de prednisolona	1108043-02	13
Euro OTC	Acetato de prednisolona	1203028-03	1
Euro OTC	Acetato de prednisolona	1209028	1
Euro OTC	Acetato de prednisolona	1209028-01	3
Euro OTC	Acetato de prednisolona	1209028-02	11
Euro OTC	Acetato de prednisolona	1209028-03	2
Euro OTC	Acetato de prednisolona	1305009-01	1
Euro OTC	Acetato de prednisolona	1306010-01	1
Euro OTC	Acetato de prednisolona	1306040-01	22
Euro OTC	Acetato de prednisolona	130604002	1
Euro OTC	Acetato de prednisolona	1306040-02	14
Euro OTC	Acetato de prednisolona	1306040-03	1
Euro OTC	Acetato de prednisolona	1306040-1	1
Euro OTC	Acetato de prednisolona	13262601	1
Euro OTC	Acetato de prednisolona	13262606	1
Euro OTC	Acetato de prednisolona	1406012-02	1
Euro OTC	Acetato de prednisolona	1406014-01	17
Euro OTC	Acetato de prednisolona	1406014-02	13
Euro OTC	Acetato de prednisolona	1407010-01	1
Euro OTC	Acetato de prednisolona	14406014-02	1
Euro OTC	Acetato de prednisolona	1460614-01	1
Euro OTC	Acetato de prednisolona	1501036	1
Euro OTC	Acetato de prednisolona	150103601	3
Euro OTC	Acetato de prednisolona	1501036-01	20
Euro OTC	Acetato de prednisolona	150103602	1
Euro OTC	Acetato de prednisolona	1501036-02	35
Euro OTC	Acetato de prednisolona	151202001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Acetato de prednisolona	1512020-01	34
Euro OTC	Acetato de prednisolona	1607010	1
Euro OTC	Acetato de prednisolona	160701001	2
Euro OTC	Acetato de prednisolona	1607010-01	98
Euro OTC	Acetato de prednisolona	1607010-10	1
Euro OTC	Acetato de prednisolona	161005PA	1
Euro OTC	Acetato de prednisolona	170104-02	1
Euro OTC	Acetato de prednisolona	1701041	2
Euro OTC	Acetato de prednisolona	170104101	3
Euro OTC	Acetato de prednisolona	1701041-01	52
Euro OTC	Acetato de prednisolona	170104102	1
Euro OTC	Acetato de prednisolona	1701041-02	53
Euro OTC	Acetato de prednisolona	1701041-03	8
Euro OTC	Acetato de prednisolona	170413PA/1607010-01	1
Euro OTC	Acetato de prednisolona	17086101	1
Euro OTC	Acetato de prednisolona	18004403	1
Euro OTC	Acetato de prednisolona	1805009	5
Euro OTC	Acetato de prednisolona	1805009-01	57
Euro OTC	Acetato de prednisolona	1805009-02	39
Euro OTC	Acetato de prednisolona	1805009-03	14
Euro OTC	Acetato de prednisolona	18050099-01	1
Euro OTC	Acetato de prednisolona	180509-01	1
Euro OTC	Acetato de prednisolona	180509-03	1
Euro OTC	Acetato de prednisolona	18067302	1
Euro OTC	Acetato de prednisolona	18067320	1
Euro OTC	Acetato de prednisolona	1903031	6
Euro OTC	Acetato de prednisolona	190303101	4
Euro OTC	Acetato de prednisolona	1903031-01	92
Euro OTC	Acetato de prednisolona	190303102	1
Euro OTC	Acetato de prednisolona	1903031-02	27
Euro OTC	Acetato de prednisolona	1911014	1
Euro OTC	Acetato de prednisolona	191101401	3
Euro OTC	Acetato de prednisolona	1911014-01	105
Euro OTC	Acetato de prednisolona	191101402	1
Euro OTC	Acetato de prednisolona	1911014-02	43
Euro OTC	Acetato de prednisolona	1911014-03	1
Euro OTC	Acetato de prednisolona	191104-01	1
Euro OTC	Acetato de prednisolona	191104-02	1
Euro OTC	Acetato de prednisolona	19111014	1
Euro OTC	Acetato de prednisolona	2(1903031-01)	1
Euro OTC	Acetato de prednisolona	200540	2
Euro OTC	Acetato de prednisolona	2010010-01	1
Euro OTC	Acetato de prednisolona	201001601	4
Euro OTC	Acetato de prednisolona	2010016-01	94
Euro OTC	Acetato de prednisolona	20-10016-01	1
Euro OTC	Acetato de prednisolona	2201028	1
Euro OTC	Acetato de prednisolona	2201028-01	39
Euro OTC	Acetato de prednisolona	220128-01	1
Euro OTC	Acetato de prednisolona	221028-01	1
Euro OTC	Acetato de prednisolona	2215I-02106	1
Euro OTC	Acetato de prednisolona	2413Q02106	1
Euro OTC	Acetato de prednisolona	2507212106	1
Euro OTC	Acetato de prednisolona	2517Q-02106	1
Euro OTC	Acetato de prednisolona	2714U-02106	1
Euro OTC	Acetato de prednisolona	289295	1
Euro OTC	Acetato de prednisolona	2918E-02106	1
Euro OTC	Acetato de prednisolona	5012I-02106	1
Euro OTC	Acetato de prednisolona	514U2106	1
Euro OTC	Acetato de prednisolona	711212106	1
Euro OTC	Acetato de prednisolona	911014-021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Acetato de prednisolona	K07A20140304M	1
Euro OTC	Acetato de prednisolona	K07A20170803M	1
Euro OTC	Acetato de prednisolona	K07A20190507	7
Euro OTC	Acetato de prednisolona	K07D20161003M	1
Euro OTC	Acetato de prednisolona	P161	1
Euro/ Gehe	Acetato de prednisolona	1911014-02	1
EUro/AHD	Acetato de prednisolona	1306040-01	1
EUro/AHD	Acetato de prednisolona	1306040-02	1
Euro/Phönix	Acetato de prednisolona	1805009-02	1
Euro/Sana	Acetato de prednisolona	1805009-01	1
Euro/Sanacorp	Acetato de prednisolona	1805009-02	1
Euro/Sanacorp	Acetato de prednisolona	1911014-01	2
Euro/Sanacorp	Acetato de prednisolona	20J01-F12-374299	1
EuRoh/ Gehe	Acetato de prednisolona	18004402	1
Euroo/Gehe	Acetato de prednisolona	1501036-02	1
fagro	Acetato de prednisolona	15B03-B05-302564	1
Fagron	Acetato de prednisolona		3
Fagron	Acetato de prednisolona	113Q-02106	1
Fagron	Acetato de prednisolona	115B03-B05-308582	1
Fagron	Acetato de prednisolona	11A31-N03	1
Fagron	Acetato de prednisolona	11I09N-08	1
Fagron	Acetato de prednisolona	11I09-N08	1
Fagron	Acetato de prednisolona	12324502	1
Fagron	Acetato de prednisolona	12C19-N03	4
Fagron	Acetato de prednisolona	12C19-NO3	1
Fagron	Acetato de prednisolona	12G25-N05	5
Fagron	Acetato de prednisolona	12h14-n07	1
Fagron	Acetato de prednisolona	12H14-N07	4
Fagron	Acetato de prednisolona	12H14-NO7	1
Fagron	Acetato de prednisolona	12J10/N05	1
Fagron	Acetato de prednisolona	12J10-N05	1
Fagron	Acetato de prednisolona	12k20-b04293971	1
Fagron	Acetato de prednisolona	12L05-N01	5
Fagron	Acetato de prednisolona	12L11-B04-286905	1
Fagron	Acetato de prednisolona	12L11-B40	1
Fagron	Acetato de prednisolona	12L11-B40-286905	13
Fagron	Acetato de prednisolona	12L11-B40-286915	2
Fagron	Acetato de prednisolona	13262605	1
Fagron	Acetato de prednisolona	13a07n07	1
Fagron	Acetato de prednisolona	13A07-N07	7
Fagron	Acetato de prednisolona	13D03-N06	1
Fagron	Acetato de prednisolona	13K20-B04-289494	2
Fagron	Acetato de prednisolona	13K20-B04-289495	3
Fagron	Acetato de prednisolona	13K20-B04-293970	1
Fagron	Acetato de prednisolona	13K20-B04-293971	3
Fagron	Acetato de prednisolona	14380909	1
Fagron	Acetato de prednisolona	14D04-B03-299294	4
Fagron	Acetato de prednisolona	14D04B03299295	1
Fagron	Acetato de prednisolona	14G30-B13	2
Fagron	Acetato de prednisolona	14G30-B13-299293	5
Fagron	Acetato de prednisolona	14G30-B13-302562	1
Fagron	Acetato de prednisolona	15/23-B04-334668	1
Fagron	Acetato de prednisolona	15/23-B04-334688	1
Fagron	Acetato de prednisolona	15/23-B04-334702	1
Fagron	Acetato de prednisolona	15/23-B04-336299	1
Fagron	Acetato de prednisolona	15/23-B04-341793	1
Fagron	Acetato de prednisolona	15/23-B04-345785	1
Fagron	Acetato de prednisolona	15055201	1
Fagron	Acetato de prednisolona	1523-B04	1
Fagron	Acetato de prednisolona	1523-b04-345785	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Acetato de prednisolona	15-23-B04-346700	1
Fagron	Acetato de prednisolona	15398401	1
Fagron	Acetato de prednisolona	15803-B05	1
Fagron	Acetato de prednisolona	15B03_B05_302564	2
Fagron	Acetato de prednisolona	15B03-B05	3
Fagron	Acetato de prednisolona	15b03-b05-302564	1
Fagron	Acetato de prednisolona	15B03B05302564	1
Fagron	Acetato de prednisolona	15B03-B05-302564	17
Fagron	Acetato de prednisolona	15B03-B05-302566	3
Fagron	Acetato de prednisolona	15B03-B05-308574	2
Fagron	Acetato de prednisolona	15B03-B05-308582	7
Fagron	Acetato de prednisolona	15BO3-B05-302564	1
Fagron	Acetato de prednisolona	15F29-B07-317179	4
Fagron	Acetato de prednisolona	15F29-B07-321001	2
Fagron	Acetato de prednisolona	15F29-B07-323268	2
Fagron	Acetato de prednisolona	15I23-B04	2
Fagron	Acetato de prednisolona	15I23-B04-327929	1
Fagron	Acetato de prednisolona	15I23-B04-331154	8
Fagron	Acetato de prednisolona	15I23-B04-334688	1
Fagron	Acetato de prednisolona	15I23-B04-334702	3
Fagron	Acetato de prednisolona	15i23-b04-336299	1
Fagron	Acetato de prednisolona	15I23-B04-336299	2
Fagron	Acetato de prednisolona	15I23-B04-340335	1
Fagron	Acetato de prednisolona	15I23-B04-341793	2
Fagron	Acetato de prednisolona	15I23-B04-345785	2
Fagron	Acetato de prednisolona	15I23-B04-346700	1
Fagron	Acetato de prednisolona	15l2351-b04-336299	1
Fagron	Acetato de prednisolona	15l23-B04-324088	1
Fagron	Acetato de prednisolona	15l23-B04-327929	1
Fagron	Acetato de prednisolona	15l23-B04-341793	1
Fagron	Acetato de prednisolona	15l23-B4-334688	1
Fagron	Acetato de prednisolona	1607010-01	1
Fagron	Acetato de prednisolona	17189601	1
Fagron	Acetato de prednisolona	1805009-01	1
Fagron	Acetato de prednisolona	180713a	1
Fagron	Acetato de prednisolona	1911014-01	1
Fagron	Acetato de prednisolona	19C28-B02-361965	1
Fagron	Acetato de prednisolona	19J08	1
Fagron	Acetato de prednisolona	19J08-F02	2
Fagron	Acetato de prednisolona	19J08-F02-365546	1
Fagron	Acetato de prednisolona	19J08-F02-366051	1
Fagron	Acetato de prednisolona	200540-0013	1
Fagron	Acetato de prednisolona	20C06-F02	3
Fagron	Acetato de prednisolona	20C06-F02-370047	2
Fagron	Acetato de prednisolona	20C06-F02-370049	4
Fagron	Acetato de prednisolona	20J01-F12	1
Fagron	Acetato de prednisolona	20J01-F12-374299	2
Fagron	Acetato de prednisolona	20J01-F12-374300	3
Fagron	Acetato de prednisolona	20J01-F12-374302	1
Fagron	Acetato de prednisolona	20J02-F12	1
Fagron	Acetato de prednisolona	21K18-B05-220957	3
Fagron	Acetato de prednisolona	5444	1
Fagron	Acetato de prednisolona	6082013D	1
Fagron	Acetato de prednisolona	F02-3700409	1
Fagron	Acetato de prednisolona	F12-3742909	1
Fagron	Acetato de prednisolona	F12-374299	1
Fagron	Acetato de prednisolona	F12-3743000	3
Fagron	Acetato de prednisolona	K07A20130903M	1
Fagron	Acetato de prednisolona	K07D20150105M	2
Fagron	Acetato de prednisolona	K07D20150503M	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Acetato de prednisolona	pa/m/013/19	1
Fagron	Acetato de prednisolona	PA/M/016/19	1
Fargo/Noweda	Acetato de prednisolona	15I23-B04-345785	2
Fargo	Acetato de prednisolona	12025-N05	1
Fargon	Acetato de prednisolona	13A07-N07	1
Fiebig	Acetato de prednisolona	1501036-01	1
Fiebig	Acetato de prednisolona	18067303	1
Fiebig	Acetato de prednisolona	18067307	1
Fiebig	Acetato de prednisolona	18067317	1
Finteler Apotheke	Acetato de prednisolona	16246812	1
Finteler Apotheke	Acetato de prednisolona	17086103	1
Fragron	Acetato de prednisolona	K07A20131101M	1
Gehe / EuRho	Acetato de prednisolona	1911014-02	1
GEHE 03.07.2014	Acetato de prednisolona	13262605	1
Gehe amax	Acetato de prednisolona	17086101	2
Gehe amax	Acetato de prednisolona	1911014-01	1
Gehe Rostock	Acetato de prednisolona	2201028	1
Gehe/Apo-Ident	Acetato de prednisolona	1701041-02	2
Gehe/EuRho 10.09.2021	Acetato de prednisolona	2010016-01	2
Gehe/EuRo	Acetato de prednisolona	1701041-02	1
Gehe/EuRoh	Acetato de prednisolona	191101402	1
Gehe	Acetato de prednisolona	1209028-01	1
Gehe	Acetato de prednisolona	1209028-02	2
Gehe	Acetato de prednisolona	12H14-N07	1
Gehe	Acetato de prednisolona	13262609	1
Gehe	Acetato de prednisolona	1406014-01	1
Gehe	Acetato de prednisolona	1501036-02	2
Gehe	Acetato de prednisolona	1512020-01	1
Gehe	Acetato de prednisolona	15B03-B05-302566	1
Gehe	Acetato de prednisolona	15I23-B04-327929	1
Gehe	Acetato de prednisolona	160701001	1
Gehe	Acetato de prednisolona	1607010-01	1
Gehe	Acetato de prednisolona	16246803	2
Gehe	Acetato de prednisolona	16246806	2
GEHE	Acetato de prednisolona	16246807	1
Gehe	Acetato de prednisolona	16246812	1
Gehe	Acetato de prednisolona	1701041-01	2
Gehe	Acetato de prednisolona	1701041-02	2
Gehe	Acetato de prednisolona	17185601	1
GEHE	Acetato de prednisolona	17185601	1
Gehe	Acetato de prednisolona	17185602	2
Gehe	Acetato de prednisolona	1805009-01	1
Gehe	Acetato de prednisolona	1805009-03	1
GEHE	Acetato de prednisolona	18067302	1
Gehe	Acetato de prednisolona	18067303	2
Gehe	Acetato de prednisolona	18067309	1
Gehe	Acetato de prednisolona	18067310	1
Gehe	Acetato de prednisolona	18067314	2
Gehe	Acetato de prednisolona	1903031-01	1
GEHE	Acetato de prednisolona	1903031-01	1
Gehe	Acetato de prednisolona	1911014-01	2
Gehe	Acetato de prednisolona	192969004	1
Gehe	Acetato de prednisolona	2010016-01	2
Gehe	Acetato de prednisolona	2201028-01	2
Gehe	Acetato de prednisolona	2201028-02	1
Hanan/Phoenix	Acetato de prednisolona	K07A20180303M	1
Henan / Gehe	Acetato de prednisolona	20001950002	2
Henan Lihua Pharm/AHD	Acetato de prednisolona	18067310	1
Henan Lihua Pharmace...	Acetato de prednisolona	14G30-B13	1
Henan Lihua Pharmace...	Acetato de prednisolona	1903031-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Henan Lihua Pharmace...	Acetato de prednisolona	2010016-01	1
Henan Lihua/Phönix	Acetato de prednisolona	1911014-02	1
Henan Lihus Pharm. C...	Acetato de prednisolona	1903031-0	1
Henan Lihus Pharm. C...	Acetato de prednisolona	1911014-02	1
Henan LP / Gehe	Acetato de prednisolona	192969005	1
Henan/Alliance	Acetato de prednisolona	18067314	1
Henan/Noweda	Acetato de prednisolona	K07A20170803M	1
Henan/Noweda	Acetato de prednisolona	K07A20190507	2
Henan/Phoenix	Acetato de prednisolona	K07A20180603M	2
Kehr	Acetato de prednisolona	1406014-01	1
L30	Acetato de prednisolona	18004402	1
L30	Acetato de prednisolona	18067303	1
Lihua Pharm	Acetato de prednisolona	K07A20140302M	1
Lihua Pharma	Acetato de prednisolona	1406014-01	1
Max Jenne/Euro	Acetato de prednisolona	1911014-01	1
Nachprüfung	Acetato de prednisolona	1019I-02106	1
Nachprüfung	Acetato de prednisolona	2082019-2	1
NMoweda	Acetato de prednisolona	2201028-01	1
Noweda 13.11. EK 17,81	Acetato de prednisolona	ko7A20200901	2
Noweda 18.05.2015	Acetato de prednisolona	14D04-B03-299294	1
Noweda Taucha	Acetato de prednisolona	190303101	1
Noweda/EuRo	Acetato de prednisolona	1607010-01	1
Noweda	Acetato de prednisolona	1209028-01	1
Noweda	Acetato de prednisolona	12324506	1
Noweda	Acetato de prednisolona	12L11-B40-286905	1
noweda	Acetato de prednisolona	14175513	1
Noweda	Acetato de prednisolona	15055202	1
Noweda	Acetato de prednisolona	1523-B04-334688	1
Noweda	Acetato de prednisolona	15398303	1
Noweda	Acetato de prednisolona	1701041-02	1
Noweda	Acetato de prednisolona	17010410203707556	1
Noweda	Acetato de prednisolona	17185602	1
Noweda	Acetato de prednisolona	1805009-01	1
Noweda	Acetato de prednisolona	18067302	1
Noweda	Acetato de prednisolona	18067325	1
Noweda	Acetato de prednisolona	1903031-01	2
Noweda	Acetato de prednisolona	1903301_01	1
Noweda	Acetato de prednisolona	191101401	1
Noweda	Acetato de prednisolona	1911014-01	5
Noweda	Acetato de prednisolona	1911014-02	3
Noweda	Acetato de prednisolona	192969003	1
Noweda	Acetato de prednisolona	19J08-F02-366051	1
Noweda	Acetato de prednisolona	2010016-01	2
Noweda	Acetato de prednisolona	22001230004	1
Noweda	Acetato de prednisolona	22001230007	1
Noweda	Acetato de prednisolona	2201028	1
Noweda	Acetato de prednisolona	2201028-02	2
Noweda	Acetato de prednisolona	230901301	1
Noweda	Acetato de prednisolona	K07D20150105M	1
Phoenix	Acetato de prednisolona	12L11-B40-286905	1
Phoenix	Acetato de prednisolona	14380905	1
Phoenix	Acetato de prednisolona	17185601	1
Phoenix	Acetato de prednisolona	17185602	2
Phoenix	Acetato de prednisolona	18067310	1
Phoenix	Acetato de prednisolona	18067314	2
Phoenix	Acetato de prednisolona	1911014-01	1
Phoenix	Acetato de prednisolona	1911014-02	1
Phoenix	Acetato de prednisolona	192969004	2
Phoenix	Acetato de prednisolona	20001950001	1
Phoenix	Acetato de prednisolona	20003843003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Acetato de prednisolona	200540	1
Phoenix	Acetato de prednisolona	2010016-01	1
Phoenix	Acetato de prednisolona	2010016-1	1
Phoenix	Acetato de prednisolona	21001844002	1
Phoenix	Acetato de prednisolona	22001230003	1
Phoenix	Acetato de prednisolona	2200123004	1
Phoenix	Acetato de prednisolona	3369	1
Phönix 09.05.2019	Acetato de prednisolona	1805009-02	1
Phönix 23.08.2019	Acetato de prednisolona	18067320	1
Phönix Gotha	Acetato de prednisolona	18067310	1
Phönix Gotha	Acetato de prednisolona	18067314	1
Phönix W.E:17.03.18 ...	Acetato de prednisolona	17185601	1
Phönix, Avik Pharmac...	Acetato de prednisolona	19J08-F02-365543	1
Phönix	Acetato de prednisolona	11158008	1
Phönix	Acetato de prednisolona	1209028-02	1
Phönix	Acetato de prednisolona	12324506	1
Phönix	Acetato de prednisolona	13262605	2
phönix	Acetato de prednisolona	14380902	2
phönix	Acetato de prednisolona	14380910	1
phönix	Acetato de prednisolona	1438910	1
phönix	Acetato de prednisolona	1512020-01	1
phönix	Acetato de prednisolona	15398303	1
Phönix	Acetato de prednisolona	15398303	1
phönix	Acetato de prednisolona	15398402	1
phönix	Acetato de prednisolona	16246803	3
Phönix	Acetato de prednisolona	16246804	1
phönix	Acetato de prednisolona	16246806	1
phönix	Acetato de prednisolona	16246807	1
Phönix	Acetato de prednisolona	17185602	2
Phönix	Acetato de prednisolona	17185603	1
Phönix	Acetato de prednisolona	1805009-01	1
Phönix	Acetato de prednisolona	18067303	3
Phönix	Acetato de prednisolona	18067317	1
Phönix	Acetato de prednisolona	18067320	1
Phönix	Acetato de prednisolona	1903031-01	1
Phönix	Acetato de prednisolona	192969004	1
Phönix	Acetato de prednisolona	192969005	2
Phönix	Acetato de prednisolona	20001950001	1
Phönix	Acetato de prednisolona	20003843003	1
Phönix	Acetato de prednisolona	2001950001	1
Phönix	Acetato de prednisolona	21001844002	2
Phönix	Acetato de prednisolona	2200001230007	1
Phönix_28.11.2018	Acetato de prednisolona	1805009-01	2
PhönixWE:10.02.2017 ...	Acetato de prednisolona	16246806	1
Post Apotheke	Acetato de prednisolona	18067301	1
Röntgen	Acetato de prednisolona	1911014-02	1
Röntgen	Acetato de prednisolona	192969004	1
Sana	Acetato de prednisolona	15L23B04345785	1
Sanacorp 07.06.2019 ...	Acetato de prednisolona	18067307	1
Sanacorp 14.03.2017 ...	Acetato de prednisolona	16246802	1
Sanacorp	Acetato de prednisolona	12091808	1
sanacorp	Acetato de prednisolona	14380909	1
Sanacorp	Acetato de prednisolona	15055206	1
Sanacorp	Acetato de prednisolona	15398408	1
Sanacorp	Acetato de prednisolona	15123-B04-334688	2
Sanacorp	Acetato de prednisolona	15123-B04-341793	1
Sanacorp	Acetato de prednisolona	17086104	1
Sanacorp	Acetato de prednisolona	17185601	1
Sanacorp	Acetato de prednisolona	17185602	1
Sanacorp	Acetato de prednisolona	17185603	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Acetato de prednisolona	18067303	2
Sanacorp	Acetato de prednisolona	18067307	1
Sanacorp	Acetato de prednisolona	18067309	2
Sanacorp	Acetato de prednisolona	19003031-01	1
Sanacorp	Acetato de prednisolona	1911014-01	1
sanacorp	Acetato de prednisolona	19J08-F02-365542	1
sanacorp	Acetato de prednisolona	200607	1
Sanacorp	Acetato de prednisolona	20J01-F12-3743000	1
Sanacorp	Acetato de prednisolona	21001844012	1
Sanacorp	Acetato de prednisolona	22001230001	1
Sanacorp	Acetato de prednisolona	22001230002	1
Sanacorp	Acetato de prednisolona	22001230003	1
Sanacorp	Acetato de prednisolona	2201028-01	1
Sanacorp	Acetato de prednisolona	K07A20200902	1
Sanofi / Gehe	Acetato de prednisolona	16246801	1
Spangro 08.05.2018	Acetato de prednisolona	17185601	1
Spangro 30.5.14	Acetato de prednisolona	13262606	1
Symbiotica Spec./Phönix	Acetato de prednisolona	1306040-02	1
Symbiotika/Anzag	Acetato de prednisolona	1306040-01	1
VDL;7,15EUR, 21:06:14	Acetato de prednisolona	13262602	1
Wolf-Apotheke	Acetato de prednisolona	14380911	1

- 232 494 spectra from 1514 *Apo-Ident* customers from a total of 48 836 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetato de prednisolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetato de prednisolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	685	0	152 277
Type B	0	1098	0	200 986
Type C	0	3561	12	232 494

The substance/substance group *Acetato de prednisolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1241 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4536 %)
Type C	100.0000 % (> 99.9007 %)	99.6641 % (> 99.5802 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20784	22297	8,81	86,59
20795	22297	9,70	79,19
20877	22297	10,77	84,72
21096	21530	5,85	80,88
21448	22297	7,36	82,87
21450	22297	7,26	81,58
21530	21530	0,00	78,70
22297	22297	0,00	83,84
24587	22297	14,34	77,16
25525	25525	0,00	79,38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de sódio tri-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20984-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de sódio tri-hidratado; Natrii acetas trihydricum

Special notes

When selecting the *Acetato de sódio tri-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de sódio tri-hidratado	6	10	34

Second-stage model

For differentiation of the substance/substance group *Acetato de sódio tri-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de sódio tri-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	56,86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de sódio tri-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de sódio tri-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetato de sódio tri-hidratado	12316506	20984	40	1402111
Caelo	Acetato de sódio tri-hidratado	13411404	21441	60	20140113
Caelo	Acetato de sódio tri-hidratado	172003	23812	40	20171107*
Euro OTC	Acetato de sódio tri-hidratado	1507020	21861	60	20150723*
Euro OTC	Acetato de sódio tri-hidratado	1706008	23547	40	20170710*
Euro OTC	Acetato de sódio tri-hidratado	2002041	25131	40	20200331*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 6 reference samples from the substance/substance group *Acetato de sódio tri-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 490 spectra of 13 reference samples from the substance/substance group *Acetato de sódio tri-hidratado*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetato de sódio tri-hidratado	163007	22760	40
Caelo	Acetato de sódio tri-hidratado	183152	24370	40
Caelo	Acetato de sódio tri-hidratado	21003448002	25983	40
Caelo	Acetato de sódio tri-hidratado	22000375	26009	40
Caelo	Acetato de sódio tri-hidratado	22003140	26478	30
Caelo	Acetato de sódio tri-hidratado	24000576	27124	40
Euro OTC	Acetato de sódio tri-hidratado	1608032	22802	40
Euro OTC	Acetato de sódio tri-hidratado	1901026	24595	40
Euro OTC	Acetato de sódio tri-hidratado	1906023	24811	40
Euro OTC	Acetato de sódio tri-hidratado	2007023	25312	40
Caelo	Acetato de sódio tri-hidratado	21003448002	25983SI	40
Caelo	Acetato de sódio tri-hidratado	22000375	26009SI	40
Caelo	Acetato de sódio tri-hidratado	22003140	26478SI	20

- 201 594 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 91 spectra from 61 *Apo-Ident* customers from 36 batches from the substance/substance group *Acetato de sódio tri-hidratado*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Acetato de sódio tri-hidratado	21003723003	1
	Acetato de sódio tri-hidratado	22000375003	1
	Acetato de sódio tri-hidratado	22000375008	1
Anzag 02.11.20 6,55EUR	Acetato de sódio tri-hidratado	220110NT	1
Caelo	Acetato de sódio tri-hidratado	10353017	1
Caelo	Acetato de sódio tri-hidratado	12027202	1
Caelo	Acetato de sódio tri-hidratado	12027217	1
Caelo	Acetato de sódio tri-hidratado	12027228	1
Caelo	Acetato de sódio tri-hidratado	12316501	1
Caelo	Acetato de sódio tri-hidratado	13295601	1
Caelo	Acetato de sódio tri-hidratado	13295606	1
Caelo	Acetato de sódio tri-hidratado	13411404	1
Caelo	Acetato de sódio tri-hidratado	13411418	2
Caelo	Acetato de sódio tri-hidratado	15118701	5
Caelo	Acetato de sódio tri-hidratado	151452009	1
Caelo	Acetato de sódio tri-hidratado	15145204	5
Caelo	Acetato de sódio tri-hidratado	15145205	1
Caelo	Acetato de sódio tri-hidratado	15145209	5
Caelo	Acetato de sódio tri-hidratado	15145218	3
Caelo	Acetato de sódio tri-hidratado	16300705	1
Caelo	Acetato de sódio tri-hidratado	16300706	5
Caelo	Acetato de sódio tri-hidratado	16300711	9
Caelo	Acetato de sódio tri-hidratado	16300712	1
Caelo	Acetato de sódio tri-hidratado	18006801	7
Caelo	Acetato de sódio tri-hidratado	18173602	3
Caelo	Acetato de sódio tri-hidratado	18315203	3
Caelo	Acetato de sódio tri-hidratado	18315208	2
Caelo	Acetato de sódio tri-hidratado	192116002	1
Caelo	Acetato de sódio tri-hidratado	21000786002	3
Caelo	Acetato de sódio tri-hidratado	21000786006	2
Caelo	Acetato de sódio tri-hidratado	21003448002	2
Caelo	Acetato de sódio tri-hidratado	22000375003	1
Caesar & Lorenz GmbH	Acetato de sódio tri-hidratado	16300706	1
Caesar & Loretz GmbH…	Acetato de sódio tri-hidratado	21003448002	1
Caesar & Loretz GmbH	Acetato de sódio tri-hidratado	192116003	1
Caesar & Loretz GmbH	Acetato de sódio tri-hidratado	21000786002	2
Caesar & Loretz GmbH	Acetato de sódio tri-hidratado	21003448002	1
Caesar & Loretz GmbH	Acetato de sódio tri-hidratado	22000375008	1
Ebert & Jacobi	Acetato de sódio tri-hidratado	15145209	1
Ebert KKH 13.10.16	Acetato de sódio tri-hidratado	15145204	1
Ebert KKH 13.10.16	Acetato de sódio tri-hidratado	15145209	1
Euro OTC	Acetato de sódio tri-hidratado	1005020V-01	1
Euro OTC	Acetato de sódio tri-hidratado	2002041-01	1
Euro OTC	Acetato de sódio tri-hidratado	2007023-01	1
Noweda	Acetato de sódio tri-hidratado	21003723003	2
Phönix Gotha	Acetato de sódio tri-hidratado	12316506	1
Sanacorp	Acetato de sódio tri-hidratado	13295601	1

- 235 976 spectra from 1515 *Apo-Ident* customers from a total of 49 222 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Acetato de sódio tri-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetato de sódio tri-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	490	0	201 594
Type C	0	91	0	235 976

The substance/substance group *Acetato de sódio tri-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7755 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.4066 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20984	20984	0,00	95,57
21441	25131	9,08	98,45
21861	21861	0,00	84,63
23547	23547	0,00	90,02
23812	23812	0,00	91,58
25131	25131	0,00	102,88

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetato de zinco di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20398-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetato de zinco di-hidratado; Zinci acetas dihydricus

Special notes

When selecting the *Acetato de zinco di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetato de zinco di-hidratado	6	3	29

Second-stage model

For differentiation of the substance/substance group *Acetato de zinco di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetato de zinco di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	93,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetato de zinco di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetato de zinco di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetato de zinco di-hidratado	15383301	22728	40	20151127
Caelo	Acetato de zinco di-hidratado	153833	23030	40	20151127*
Caelo	Acetato de zinco di-hidratado	170204	23031	40	20170126*
Caelo	Acetato de zinco di-hidratado	170204	23637	40	20172601*
Caelo	Acetato de zinco di-hidratado	19000422	25208	40	20191230*
Caelo	Acetato de zinco di-hidratado	21000302	25652	40	20210303*
Caelo	Acetato de zinco di-hidratado	22002583	26479	30	20221109*
Caelo	Acetato de zinco di-hidratado	22002583	26479SI	20	20221109*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 290 spectra of 8 reference samples from the substance/substance group *Acetato de zinco di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 672 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Acetato de zinco di-hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetato de zinco di-hidratado	17020404	23514	40
Caelo	Acetato de zinco di-hidratado	182046	24213	40
Caelo	Acetato de zinco di-hidratado	23001173	26895	40
Caelo	Acetato de zinco di-hidratado	23001173	26895SI	20

- 201 944 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 99 spectra from 82 *Apo-Ident* customers from 30 batches from the substance/substance group *Acetato de zinco di-hidratado*.

- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Acetato de zinco di-hidratado	21000302011	1
	Acetato de zinco di-hidratado	22002583004	1
	Acetato de zinco di-hidratado	22002583006	1
	Acetato de zinco di-hidratado	22002583010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acetato de zinco di-hidratado	12134801	2
Caelo	Acetato de zinco di-hidratado	12134803	1
Caelo	Acetato de zinco di-hidratado	12316401	2
Caelo	Acetato de zinco di-hidratado	12316403	2
Caelo	Acetato de zinco di-hidratado	12316404	2
Caelo	Acetato de zinco di-hidratado	12316405	1
Caelo	Acetato de zinco di-hidratado	14133201	1
Caelo	Acetato de zinco di-hidratado	15160801	1
Caelo	Acetato de zinco di-hidratado	15160804	1
Caelo	Acetato de zinco di-hidratado	15383304	1
Caelo	Acetato de zinco di-hidratado	15383306	4
Caelo	Acetato de zinco di-hidratado	15383308	2
Caelo	Acetato de zinco di-hidratado	17020403	3
Caelo	Acetato de zinco di-hidratado	17020404	3
Caelo	Acetato de zinco di-hidratado	17197601	9
Caelo	Acetato de zinco di-hidratado	17365807	1
Caelo	Acetato de zinco di-hidratado	18204604	6
Caelo	Acetato de zinco di-hidratado	18204610	1
Caelo	Acetato de zinco di-hidratado	19000422007	4
Caelo	Acetato de zinco di-hidratado	19000422011	1
Caelo	Acetato de zinco di-hidratado	20004443001	2
Caelo	Acetato de zinco di-hidratado	21000302002	2
Caelo	Acetato de zinco di-hidratado	21000302006	5
Caelo	Acetato de zinco di-hidratado	21000302011	1
Caelo	Acetato de zinco di-hidratado	22002583004	5
Caesar & Loretz GmbH…	Acetato de zinco di-hidratado	19000422011	1
Caesar & Loretz GmbH…	Acetato de zinco di-hidratado	18204610	1
Caesar & Loretz GmbH…	Acetato de zinco di-hidratado	22002583004	1
Caesar & Loretz GmbH/Kehr	Acetato de zinco di-hidratado	20004443001	1
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	18204604	2
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	19000422007	1
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	19000422011	4
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	21000302002	2
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	21000302006	4
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	21000302014	1
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	22002583004	2
Caesar & Loretz GmbH	Acetato de zinco di-hidratado	22002583006	1
Caesar/Sanacorp	Acetato de zinco di-hidratado	18204604	1
Cealo	Acetato de zinco di-hidratado	17197601	1
Euro OTC	Acetato de zinco di-hidratado	15383301	1
Gehe	Acetato de zinco di-hidratado	17020404	1
Noweda	Acetato de zinco di-hidratado	18204604	1
phönix	Acetato de zinco di-hidratado	15383301	1
Phönix	Acetato de zinco di-hidratado	17197601	1
PHÖNIX	Acetato de zinco di-hidratado	19000422011	1
Phönix	Acetato de zinco di-hidratado	2200253006	1
phönix	Acetato de zinco di-hidratado	22002583004	1
Sanacorp	Acetato de zinco di-hidratado	19000422011	1

- 235 968 spectra from 1515 *Apo-Ident* customers from a total of 49 229 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetato de zinco di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

this purpose, all relevant spectra of the various substances were compared with *Acetato de zinco di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	140	0	201 944
Type C	0	98	1	235 968

The substance/substance group *Acetato de zinco di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	98.9899 % (> 95.9596 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22728	23030	4,38	157,17
23030	23030	0,00	157,04
23031	23031	0,00	154,41
23637	23637	0,00	154,51
25208	25208	0,00	156,65
25652	25652	0,00	152,21
26479	26479	0,00	152,69

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetilcisteína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20040-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetilcisteína; N-acetilcisteína

Special notes

When selecting the *Acetilcisteína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Acetilcisteína	7	15	46

Second-stage model

For differentiation of the substance/substance group *Acetilcisteína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Acetilcisteína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	116,28	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Acetilcisteína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Acetilcisteína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetilcisteína	12299020	21315	40	20121026
Caelo	Acetilcisteína	161398	22469	60	20160520*
Euro OTC	Acetilcisteína	1208026-01	21628	60	20121116
Euro OTC	Acetilcisteína	1510016	22228	60	20151116*
Euro OTC	Acetilcisteína	1610011	22854	40	20161107*
Euro OTC	Acetilcisteína	2202014	26090	40	20220512*
Fagron	Acetilcisteína	15C16-B06-308039	22886	40	20150402

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 340 spectra of 7 reference samples from the substance/substance group *Acetilcisteína*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 690 spectra of 19 reference samples from the substance/substance group *Acetilcisteína*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetilcisteína	163340	23035	40
Caelo	Acetilcisteína	20004543008	25989	40
Caelo	Acetilcisteína	22001099	26240	40
Euro OTC	Acetilcisteína	1801037	23956	40
Euro OTC	Acetilcisteína	1809026	24302	40
Euro OTC	Acetilcisteína	1907008	24837	40
Euro OTC	Acetilcisteína	1911003	24981	40
Euro OTC	Acetilcisteína	2003061	25315	40
Euro OTC	Acetilcisteína	2010011	25524	40
Euro OTC	Acetilcisteína	2208019	26340	40
Euro OTC	Acetilcisteína	2301028	26600	40
Euro OTC	Acetilcisteína	2411002	27465	30
Fagron	Acetilcisteína	18B01-B04-357511	24703	40
Fagron	Acetilcisteína	18K06-B02-363236	25043	40
Fagron	Acetilcisteína	22G22-B02-227323	26984	40
Caelo	Acetilcisteína	20004543008	25989SI	40
Caelo	Acetilcisteína	22001099	26240SI	20
Euro OTC	Acetilcisteína	2202014	26090SI†	20
Euro OTC	Acetilcisteína	2208019	26340SI	20

- 201 394 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 89 spectra from 71 *Apo-Ident* customers from 47 batches from the substance/substance group *Acetilcisteína*.
- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Acetilcisteína	20004543006	1
	Acetilcisteína	22001099005	2
	Acetilcisteína	22001099009	1
	Acetilcisteína	2208019-03	1
Caelo	Acetilcisteína	1011171701	1
Caelo	Acetilcisteína	10230713	1
Caelo	Acetilcisteína	12299004	1
Caelo	Acetilcisteína	12299021	1
Caelo	Acetilcisteína	12299027	1
Caelo	Acetilcisteína	130702601	1
Caelo	Acetilcisteína	15114007	2
Caelo	Acetilcisteína	15114013	2
Caelo	Acetilcisteína	16139802	2
Caelo	Acetilcisteína	16139808	1
Caelo	Acetilcisteína	16334006	7
Caelo	Acetilcisteína	16334007	1
Caelo	Acetilcisteína	17357305	3
Caelo	Acetilcisteína	18180402	1
Caelo	Acetilcisteína	18180405	3
Caelo	Acetilcisteína	18180409	1
Caelo	Acetilcisteína	18180412	3
Caelo	Acetilcisteína	18180421	1
Caelo	Acetilcisteína	192757006	4
Caelo	Acetilcisteína	20004543009	1
Caesar & Loretz GmbH...	Acetilcisteína	18180412	1
Caesar & Loretz GmbH/sana	Acetilcisteína	181804	1
Caesar & Loretz GmbH...	Acetilcisteína	16334006	1
Caesar & Loretz GmbH	Acetilcisteína	18180412	2
Caesar & Loretz GmbH	Acetilcisteína	20004543004	1
Caesar & Loretz GmbH	Acetilcisteína	20004543006	1
EuRho	Acetilcisteína	2010011-02	2
Euro OTC	Acetilcisteína	120802601	2
Euro OTC	Acetilcisteína	12299010	1
Euro OTC	Acetilcisteína	1307026-01	1
Euro OTC	Acetilcisteína	1505011-01	1
Euro OTC	Acetilcisteína	1510016-01	3
Euro OTC	Acetilcisteína	1610011-01	1
Euro OTC	Acetilcisteína	1610011-02	1
Euro OTC	Acetilcisteína	180103701	1
Euro OTC	Acetilcisteína	1809026-01	2
Euro OTC	Acetilcisteína	1911003-02	5
Euro OTC	Acetilcisteína	192757006	1
Euro OTC	Acetilcisteína	2010011-01	1
Euro OTC	Acetilcisteína	2010011-02	1
Fagron	Acetilcisteína	13A22N07	1
Fagron	Acetilcisteína	14C28-B05-292386	1
Fagron	Acetilcisteína	21D22-B04-213886	1
Fargon	Acetilcisteína	20G17-F01-373416	3
Farmalabor	Acetilcisteína	P1701913-003	1
Gehe	Acetilcisteína	16139813	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
gehe	Acetilcisteína	190700801	1
phar	Acetilcisteína	1610011-02	1
PharmaZell GmbH/Noweda	Acetilcisteína	1911003-02	1
Phoenix 06.06.2014	Acetilcisteína	1208026-01	1
Phoenix goettin	Acetilcisteína	1208026-01	1
Phönix	Acetilcisteína	1208026	1
Sanacorp 07.03.2016 ...	Acetilcisteína	15114007	1
Sanacorp	Acetilcisteína	18180405	1

- 235 978 spectra from 1515 *Apo-Ident* customers from a total of 49 212 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acetilcisteína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acetilcisteína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	690	0	201 394
Type C	0	89	0	235 978

The substance/substance group *Acetilcisteína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1304 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.2584 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21315	22228	15,34	213,83
21628	22469	12,38	196,88
22228	22228	0,00	214,73
22469	22469	0,00	199,19
22854	22854	0,00	215,45
22886	22228	13,62	216,96
26090	26090	0,00	226,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Aciclovir**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21677-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Aciclovir; Aciclovirum

Special notes

When selecting the *Aciclovir* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Aciclovir	6	3	25

Second-stage model

For differentiation of the substance/substance group *Aciclovir* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Aciclovir* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	86,41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Aciclovir* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Aciclovir*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Aciclovir	13B04-B40-294559	21677	60	AR-15-FG-002570-01
Fagron	Aciclovir	13B04-B40-302333	21761	60	20131217
Fagron	Aciclovir	14G07-B05-296462	21831	60	20140728
Fagron	Aciclovir	19I17-F02-366255	25064	40	20191202
Fagron	Aciclovir	24C11-B01-236108	27381	40	20240418
Gatt-Koller	Aciclovir	22J01376	27099	30	20220804

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 290 spectra of 6 reference samples from the substance/substance group *Aciclovir*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 672 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 7 reference samples from the substance/substance group *Aciclovir*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Aciclovir	15A15-B10-323362	22938	40
Fagron	Aciclovir	18I18-B04-356027	24570	40
Fagron	Aciclovir	22A15-B02-222370	26290	40
Fagron	Aciclovir	15A15-B10-323362	22939	40
Fagron	Aciclovir	22A15-B02-222370	26290SI	20
Fagron	Aciclovir	24C11-B01-236108	27381SI†	20
Gatt-Koller	Aciclovir	22J01376	27099SI†	20

- 201 864 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 47 spectra from 31 *Apo-Ident* customers from 28 batches from the substance/substance group *Aciclovir*.
- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Aciclovir	F02-3709204	1
Caelo	Aciclovir	18118-B04-355420	1
Fagron	Aciclovir	13B04-B40-288651	1
Fagron	Aciclovir	146501524	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Aciclovir	14g07-b05-296462	1
Fagron	Aciclovir	15A15-B10-307743	1
Fagron	Aciclovir	15A15-B10-315379	13
Fagron	Aciclovir	15A15-B10-323362	1
Fagron	Aciclovir	15AS15-B10-307743	1
Fagron	Aciclovir	16GK09-B05-332754	1
Fagron	Aciclovir	16K09-B05-328196	4
Fagron	Aciclovir	17G11-B01-339460	1
Fagron	Aciclovir	17G11-B01-342081	1
Fagron	Aciclovir	18/18-B04-358573	1
Fagron	Aciclovir	18/18-B24-358573	1
Fagron	Aciclovir	18I18-B04-355420	1
Fagron	Aciclovir	18I18-B04-358573	1
Fagron	Aciclovir	19/17-F02	1
Fagron	Aciclovir	19/17-F02-366256	1
Fagron	Aciclovir	19I17-F02-366255	1
Fagron	Aciclovir	19I17-F02-366256	2
Fagron	Aciclovir	19i17-F02-367853	1
Fagron	Aciclovir	19I17-F02-367853	2
Fagron	Aciclovir	19I17-FO2-366256	1
Fagron	Aciclovir	19l17-F02	1
Fagron	Aciclovir	ACV1019008	3
Fagron	Aciclovir	ACV1116001	1
Fagron	Aciclovir	F02-3678503	1

- 236 020 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Aciclovir* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Aciclovir* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	220	0	201 864
Type C	0	47	0	236 020

The substance/substance group *Aciclovir* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 87.2340 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21677	21677	0,00	204,64
21761	21677	7,32	203,16
21831	21677	17,73	204,68
25064	21677	14,62	200,89
27099	21677	14,49	204,52
27381	21677	8,58	200,89

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido 4-aminobenzoico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005947-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido 4-aminobenzoico; Acidum 4-aminobenzoicum

Special notes

When selecting the *Ácido 4-aminobenzoico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido 4-aminobenzoico	4	1	0

Second-stage model

For differentiation of the substance/substance group *Ácido 4-aminobenzoico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido 4-aminobenzoico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	177,78	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido 4-aminobenzoico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido 4-aminobenzoico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ácido 4-aminobenzoico	2111019	25867	50	20211208*
Euro OTC	Ácido 4-aminobenzoico	2203029	26050	40	20220408*
Euro OTC	Ácido 4-aminobenzoico	2205024	26207	40	20220620*
Euro OTC	Ácido 4-aminobenzoico	2205024	26207SI	20	20220620*
Euro OTC	Ácido 4-aminobenzoico	2302016	26754	40	20230511*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 190 spectra of 5 reference samples from the substance/substance group *Ácido 4-aminobenzoico*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 772 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 4 reference samples from the substance/substance group *Ácido 4-aminobenzoico*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido 4-aminobenzoico	2008012	25394	40
Euro OTC	Ácido 4-aminobenzoico	2111019	25867SI†	10
Euro OTC	Ácido 4-aminobenzoico	2203029	26050SI†	10
Euro OTC	Ácido 4-aminobenzoico	2302016	26754SI†	20

- 202 004 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ácido 4-aminobenzoico*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Ácido 4-aminobenzoico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido 4-aminobenzoico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	190	0	152 772
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Ácido 4-aminobenzoico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.8421 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25867	25867	0,00	297,23
26050	26050	0,00	297,98
26207	26207	0,00	298,54
26754	26754	0,00	297,75

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido acetilsalicílico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20449-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido acetilsalicílico; Acidum acetylsalicylicum

Special notes

When selecting the *Ácido acetilsalicílico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido acetilsalicílico	7	9	102

Second-stage model

For differentiation of the substance/substance group *Ácido acetilsalicílico* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido acetilsalicílico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	87,74	–
⋮	⋮	⋮
Ditranol	>50	17,02
Cloreto de dequalínio	>50	52,48
Salicilato de sódio	>50	69,40
Ácido benzoico	>50	79,93
Eosina amarela	>50	252,87
Cloridrato de oxitetraciclina	>50	357,71
Levotiroxina sódica	>50	683,56
Tanino	>50	1569,01

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido acetilsalicílico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido acetilsalicílico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido acetilsalicílico	13297509	21383	40	20131014
Caelo	Ácido acetilsalicílico	161316	23064	40	20160825*
Euro OTC	Ácido acetilsalicílico	1307024-01	21597	45	20130904
Euro OTC	Ácido acetilsalicílico	1407026-01	21637	60	20140801
Euro OTC	Ácido acetilsalicílico	1601042	22377	40	20160204*
Euro OTC	Ácido acetilsalicílico	1608037	22820	40	20160921*
Fagron	Ácido acetilsalicílico	14E02-B04-297099	22949	40	20140515

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 305 spectra of 7 reference samples from the substance/substance group *Ácido acetilsalicílico*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 657 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 12 reference samples from the substance/substance group *Ácido acetilsalicílico*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido acetilsalicílico	173098	23806	40
Caelo	Ácido acetilsalicílico	20003902006	25929	40
Caelo	Ácido acetilsalicílico	22000047	26011	40
Caelo	Ácido acetilsalicílico	23001248	26837	40
Caelo	Ácido acetilsalicílico	24002283	27427	40
Euro OTC	Ácido acetilsalicílico	1703010	23388	40
Euro OTC	Ácido acetilsalicílico	1805004	24120	40
Euro OTC	Ácido acetilsalicílico	1805003	24127	40
Euro OTC	Ácido acetilsalicílico	2007003	25345	40
Caelo	Ácido acetilsalicílico	20003902006	25929SI	10
Caelo	Ácido acetilsalicílico	22000047	26011SI	10
Caelo	Ácido acetilsalicílico	23001248	26837SI	20

- 201 684 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 428 spectra from 269 *Apo-Ident* customers from 105 batches from the substance/substance group *Ácido acetilsalicílico*.
- Among them are spectra of independent samples from 102 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido acetilsalicílico	2007003-03	1
	Ácido acetilsalicílico	22000047006	1
	Ácido acetilsalicílico	22000047013	2
	Ácido acetilsalicílico	22000047016	2
	Ácido acetilsalicílico	23001248003	7
	Ácido acetilsalicílico	23001248004	1
ACM	Ácido acetilsalicílico	KNC2077J14	1
ACM	Ácido acetilsalicílico	KNC2152J13	1
Alliance Healthcare	Ácido acetilsalicílico	18122605	1
Anzag	Ácido acetilsalicílico	20003902010	1
Bombastus	Ácido acetilsalicílico	1212005-01	1
Bombastus	Ácido acetilsalicílico	17023102	1
Caelo	Ácido acetilsalicílico	10099907	1
Caelo	Ácido acetilsalicílico	1061117/17023107	1
Caelo	Ácido acetilsalicílico	1110417	1
Caelo	Ácido acetilsalicílico	11257126	1
Caelo	Ácido acetilsalicílico	12212203	1
Caelo	Ácido acetilsalicílico	12212219	1
Caelo	Ácido acetilsalicílico	12212223	3
Caelo	Ácido acetilsalicílico	12212230	1
Caelo	Ácido acetilsalicílico	12212233	1
Caelo	Ácido acetilsalicílico	12212234	2
Caelo	Ácido acetilsalicílico	12212236	2
Caelo	Ácido acetilsalicílico	13297511	1
Caelo	Ácido acetilsalicílico	13324101	2
Caelo	Ácido acetilsalicílico	13324105	1
Caelo	Ácido acetilsalicílico	13324109	3
Caelo	Ácido acetilsalicílico	13324116	1
Caelo	Ácido acetilsalicílico	13324118	1
Caelo	Ácido acetilsalicílico	13324119	1
Caelo	Ácido acetilsalicílico	14189603	1
Caelo	Ácido acetilsalicílico	14250101	2
Caelo	Ácido acetilsalicílico	15081301	3
Caelo	Ácido acetilsalicílico	15081304	1
Caelo	Ácido acetilsalicílico	15081308	2
Caelo	Ácido acetilsalicílico	15081310	1
Caelo	Ácido acetilsalicílico	15122701	1
Caelo	Ácido acetilsalicílico	15334902	4
Caelo	Ácido acetilsalicílico	15334907	7
Caelo	Ácido acetilsalicílico	15334910	1
Caelo	Ácido acetilsalicílico	15334914	3
Caelo	Ácido acetilsalicílico	15334917	4
Caelo	Ácido acetilsalicílico	160104202	1
Caelo	Ácido acetilsalicílico	16131607	2
Caelo	Ácido acetilsalicílico	170230107	1
Caelo	Ácido acetilsalicílico	17023102	11
Caelo	Ácido acetilsalicílico	17023107	11
Caelo	Ácido acetilsalicílico	17023108	4
Caelo	Ácido acetilsalicílico	17023110	18
Caelo	Ácido acetilsalicílico	17023111	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido acetilsalicílico	1703010-02	1
Caelo	Ácido acetilsalicílico	1703010-03	2
Caelo	Ácido acetilsalicílico	17309801	1
Caelo	Ácido acetilsalicílico	17329204	3
Caelo	Ácido acetilsalicílico	1805004-02	2
Caelo	Ácido acetilsalicílico	18108303	2
Caelo	Ácido acetilsalicílico	18108306	2
Caelo	Ácido acetilsalicílico	18108311	1
Caelo	Ácido acetilsalicílico	18122601	2
Caelo	Ácido acetilsalicílico	18122602	13
Caelo	Ácido acetilsalicílico	18122605	16
Caelo	Ácido acetilsalicílico	18122612	14
Caelo	Ácido acetilsalicílico	18122615	3
Caelo	Ácido acetilsalicílico	1911166001	1
Caelo	Ácido acetilsalicílico	191166001	13
Caelo	Ácido acetilsalicílico	191166003	1
Caelo	Ácido acetilsalicílico	191166005	9
Caelo	Ácido acetilsalicílico	19116601	1
Caelo	Ácido acetilsalicílico	19116602	2
Caelo	Ácido acetilsalicílico	19116604	15
Caelo	Ácido acetilsalicílico	200003902006	1
Caelo	Ácido acetilsalicílico	20003902003	15
Caelo	Ácido acetilsalicílico	20003902004	2
Caelo	Ácido acetilsalicílico	20003902006	9
Caelo	Ácido acetilsalicílico	20003902008	1
Caelo	Ácido acetilsalicílico	20003902010	3
Caelo	Ácido acetilsalicílico	20003902013	6
Caelo	Ácido acetilsalicílico	2000392003	2
Caelo	Ácido acetilsalicílico	2000392006	3
Caelo	Ácido acetilsalicílico	2000392010	1
Caelo	Ácido acetilsalicílico	2003902010	1
Caelo	Ácido acetilsalicílico	22000047006	3
Caelo	Ácido acetilsalicílico	22000047013	5
Caelo	Ácido acetilsalicílico	22000047016	5
Caelo	Ácido acetilsalicílico	301115	1
Caelo	Ácido acetilsalicílico	54018122612	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	20003902013	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166001	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	22000047006	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	20003902003	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166005	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166001	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	19116604	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166001	2
Caesar & Loretz GmbH/Phoe	Ácido acetilsalicílico	20003902003	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166001	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166005	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	22000047016	1
Caesar & Loretz GmbH...	Ácido acetilsalicílico	191166001	1
Caesar & Loretz GmbH/Sana	Ácido acetilsalicílico	18122612	1
Caesar & Loretz GmbH	Ácido acetilsalicílico	15334914	1
Caesar & Loretz GmbH	Ácido acetilsalicílico	15334917	1
Caesar & Loretz GmbH	Ácido acetilsalicílico	18108311	1
Caesar & Loretz GmbH	Ácido acetilsalicílico	18122602	1
Caesar & Loretz GmbH	Ácido acetilsalicílico	18122605	4
Caesar & Loretz GmbH	Ácido acetilsalicílico	18122612	2
Caesar & Loretz GmbH	Ácido acetilsalicílico	191166001	4
Caesar & Loretz GmbH	Ácido acetilsalicílico	191166005	3
Caesar & Loretz GmbH	Ácido acetilsalicílico	19116604	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ácido acetilsalicílico	20003902003	9
Caesar & Loretz GmbH	Ácido acetilsalicílico	20003902006	5
Caesar & Loretz GmbH	Ácido acetilsalicílico	20003902010	1
Caesar & Loretz GmbH	Ácido acetilsalicílico	22000047006	4
Caesar & Loretz GmbH	Ácido acetilsalicílico	22000047013	2
Caesar & Loretz GmbH	Ácido acetilsalicílico	22000047016	1
Caesar & Loretz/Geil...	Ácido acetilsalicílico	19116604	1
Calo	Ácido acetilsalicílico	15334902	1
Cealo	Ácido acetilsalicílico	15334910	1
EuRho	Ácido acetilsalicílico	1307024-01	2
EuRho	Ácido acetilsalicílico	1407025-01	1
EuRo Gehe	Ácido acetilsalicílico	147026-01	1
Euro OTC	Ácido acetilsalicílico		1
Euro OTC	Ácido acetilsalicílico	1011015-01	1
Euro OTC	Ácido acetilsalicílico	1107007-01	1
Euro OTC	Ácido acetilsalicílico	1212005-01	3
Euro OTC	Ácido acetilsalicílico	1307024-01	6
Euro OTC	Ácido acetilsalicílico	1407025	1
Euro OTC	Ácido acetilsalicílico	1407025-01	17
Euro OTC	Ácido acetilsalicílico	1501046-01	5
Euro OTC	Ácido acetilsalicílico	1601042-02	2
Euro OTC	Ácido acetilsalicílico	1703010-03	1
Euro OTC	Ácido acetilsalicílico	1805004-01	3
Euro OTC	Ácido acetilsalicílico	1805004-02	3
Euro OTC	Ácido acetilsalicílico	18122602	1
Euro OTC	Ácido acetilsalicílico	20030611-1	1
Euro OTC	Ácido acetilsalicílico	2007003-01	2
Euro OTC	Ácido acetilsalicílico	2007003-02	1
Euro OTC	Ácido acetilsalicílico	3518A-01012	1
Euro OTC	Ácido acetilsalicílico	4017Q-01012	1
Euro OTC	Ácido acetilsalicílico	815A-01012	1
Fagron	Ácido acetilsalicílico	14B10-B02-296841	1
Gehe	Ácido acetilsalicílico	10365302	1
GEHE	Ácido acetilsalicílico	17023110	1
Gehe	Ácido acetilsalicílico	18122602	1
Gehe	Ácido acetilsalicílico	18122605	2
Gehe	Ácido acetilsalicílico	23001248003	1
L12	Ácido acetilsalicílico	15334917	1
Midas Göttingen	Ácido acetilsalicílico	191166001	1
Novacyl / Gehe	Ácido acetilsalicílico	191166001	1
Noweda	Ácido acetilsalicílico	10040403	1
Noweda	Ácido acetilsalicílico	20003902006	1
Noweda	Ácido acetilsalicílico	22000047018	1
Phoenix/Cealo	Ácido acetilsalicílico	17356301	1
Phoenix	Ácido acetilsalicílico	13324107	1
Phoenix	Ácido acetilsalicílico	19116604	1
Phoenix	Ácido acetilsalicílico	22000047013	1
Phönix	Ácido acetilsalicílico	13324114	1
Phönix	Ácido acetilsalicílico	191166005	1
Sanacorp	Ácido acetilsalicílico	1307024-01	1
Sanacorp	Ácido acetilsalicílico	13324109	1
sanacorp	Ácido acetilsalicílico	14250101	1
Sanacorp	Ácido acetilsalicílico	17329204	1
Sanacorp	Ácido acetilsalicílico	17329205	1
Stadt Apo Geesthacht	Ácido acetilsalicílico		1

- 235 639 spectra from 1515 *Apo-Ident* customers from a total of 49 157 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido acetilsalicílico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido acetilsalicílico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	305	0	152 657
Type B	0	400	0	201 684
Type C	0	408	20	235 639

The substance/substance group *Ácido acetilsalicílico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0328 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.9007 %)	95.3271 % (> 94.6262 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21383	22377	12,42	117,23
21597	22377	13,56	115,96
21637	22377	22,01	118,28
22377	22377	0,00	117,88
22820	22820	0,00	116,54
22949	22377	10,74	115,01
23064	23064	0,00	116,71

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido ascórbico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20394-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido ascórbico; Vitamina C (ácido ascórbico)

Special notes

When selecting the *Ácido ascórbico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido ascórbico	9	20	146

Second-stage model

For differentiation of the substance/substance group *Ácido ascórbico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido ascórbico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	105,18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido ascórbico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido ascórbico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido ascórbico	12350011	21317	40	20121122
Caelo	Ácido ascórbico	163452	23062	40	20170125*
Caelo	Ácido ascórbico	171358	23288	40	20170524*
Caelo	Ácido ascórbico	171358	23293	40	20170524*
Euro OTC	Ácido ascórbico	1607025	22672	40	20160801*
Euro OTC	Ácido ascórbico	1605024	22680	40	20160617*
Euro OTC	Ácido ascórbico	1609015	22789	40	20161006*
Euro OTC	Ácido ascórbico	1612018	22918	40	20170109*
Euro OTC	Ácido ascórbico	1911012	24936	40	20191204*
Fagron	Ácido ascórbico	13G29-B07	21229	40	1410500

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Ácido ascórbico*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 860 spectra of 23 reference samples from the substance/substance group *Ácido ascórbico*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido ascórbico	190262	24508	40
Caelo	Ácido ascórbico	192143	24893	40
Caelo	Ácido ascórbico	22001801	26257	40
Caelo	Ácido ascórbico	24000579	27132	40
Euro OTC	Ácido ascórbico	1703040	23128	40
Euro OTC	Ácido ascórbico	1703025	23144	40
Euro OTC	Ácido ascórbico	1707005	23553	40
Euro OTC	Ácido ascórbico	1708026	23701	40
Euro OTC	Ácido ascórbico	1710032	23891	40
Euro OTC	Ácido ascórbico	1901044	24462	40
Euro OTC	Ácido ascórbico	1903008	24634	40
Euro OTC	Ácido ascórbico	1909018	24848	40
Euro OTC	Ácido ascórbico	1911013	24975	40
Euro OTC	Ácido ascórbico	2002022	25126	40
Euro OTC	Ácido ascórbico	2002023	25154	40
Euro OTC	Ácido ascórbico	2307032	26868	40
Euro OTC	Ácido ascórbico	2307033	26874	40
Fagron	Ácido ascórbico	19G18-B03-194674	25041	40
Fagron	Ácido ascórbico	22A21-B05-218612	26155	40
Fagron	Ácido ascórbico	24C07-B16-235947	27386	40
Caelo	Ácido ascórbico	22001801	26257SI	20
Euro OTC	Ácido ascórbico	2307032	26868SI	20
Fagron	Ácido ascórbico	22A21-B05-218612	26155SI	20

- 201 224 spectra from a total of 4025 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 339 spectra from 232 *Apo-Ident* customers from 151 batches from the substance/substance group *Ácido ascórbico*.
- Among them are spectra of independent samples from 145 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido ascórbico	1210142074	1
	Ácido ascórbico	22001801006	4
	Ácido ascórbico	23000894001	5
	Ácido ascórbico	23000894006	4
	Ácido ascórbico	2307032-01	1
	Ácido ascórbico	CH1210142074	1
	Ácido ascórbico	VC2302	1
	Ácido ascórbico	VC2315	1
ACM Herba	Ácido ascórbico	KNC0385J21	3
ACM	Ácido ascórbico	Knc1035j16	1
ACM	Ácido ascórbico	KNC1035J16	2
ACM	Ácido ascórbico	KNC1488J14	6
Alliance Healthcare	Ácido ascórbico	192143005	1
alliance	Ácido ascórbico	23000894001	1
Amos Vital GmbH/Alli...	Ácido ascórbico	L1711004	1
Amos Vital GmbH	Ácido ascórbico	L1411003	1
Amos Vital	Ácido ascórbico	L1120454	1
Amos vital	Ácido ascórbico	L1501004	1
Amosvital GMBH	Ácido ascórbico	201084	1
Amosvital/Fiebig	Ácido ascórbico	L1509002	1
apoday	Ácido ascórbico	HPB1804126	1
Apolda/Noweda	Ácido ascórbico	15021548	1
Atlantic chemicals	Ácido ascórbico	DY0261921097	2
Caealo/phoen	Ácido ascórbico	2223806007	1
Caelo	Ácido ascórbico	1071404	1
Caelo	Ácido ascórbico	11208606	1
Caelo	Ácido ascórbico	1121010320	1
Caelo	Ácido ascórbico	12272601/1	1
Caelo	Ácido ascórbico	123456	2
Caelo	Ácido ascórbico	1234567	1
Caelo	Ácido ascórbico	12349909	1
Caelo	Ácido ascórbico	12350003	1
Caelo	Ácido ascórbico	12350005	2
Caelo	Ácido ascórbico	12350011	1
Caelo	Ácido ascórbico	123test	3
Caelo	Ácido ascórbico	123Test	2
Caelo	Ácido ascórbico	12456	1
Caelo	Ácido ascórbico	13341803/3	1
Caelo	Ácido ascórbico	14044701/3	1
Caelo	Ácido ascórbico	14123809	3
Caelo	Ácido ascórbico	14123910	1
Caelo	Ácido ascórbico	14123915	2
Caelo	Ácido ascórbico	14214403	1
Caelo	Ácido ascórbico	15084503	1
Caelo	Ácido ascórbico	15084507	1
Caelo	Ácido ascórbico	151214588	1
Caelo	Ácido ascórbico	153000	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido ascórbico	15300002	5
Caelo	Ácido ascórbico	15300007	8
Caelo	Ácido ascórbico	15359003	2
Caelo	Ácido ascórbico	16050403	4
Caelo	Ácido ascórbico	16345202	5
Caelo	Ácido ascórbico	16345204	1
Caelo	Ácido ascórbico	16345205	6
Caelo	Ácido ascórbico	17135803	6
Caelo	Ácido ascórbico	17233201	1
Caelo	Ácido ascórbico	17360301	8
Caelo	Ácido ascórbico	17360308	3
Caelo	Ácido ascórbico	17564875	1
Caelo	Ácido ascórbico	18030501	1
Caelo	Ácido ascórbico	18030503	1
Caelo	Ácido ascórbico	18127801	2
Caelo	Ácido ascórbico	18127805	6
Caelo	Ácido ascórbico	18127811	6
Caelo	Ácido ascórbico	1812805	1
Caelo	Ácido ascórbico	19026202	6
Caelo	Ácido ascórbico	192143002	4
Caelo	Ácido ascórbico	192143005	7
Caelo	Ácido ascórbico	192143006	1
Caelo	Ácido ascórbico	200003806007	1
Caelo	Ácido ascórbico	20000988002	1
Caelo	Ácido ascórbico	20001112002	1
Caelo	Ácido ascórbico	20001112003	4
Caelo	Ácido ascórbico	20001112033	1
Caelo	Ácido ascórbico	20003806003	3
Caelo	Ácido ascórbico	20003806005	1
Caelo	Ácido ascórbico	20003806007	3
Caelo	Ácido ascórbico	20003806018	3
Caelo	Ácido ascórbico	2061203	1
Caelo	Ácido ascórbico	21001355002	1
Caelo	Ácido ascórbico	22101302	1
Caelo	Ácido ascórbico	23000894001	1
Caelo	Ácido ascórbico	3819Q-01016	1
Caelo	Ácido ascórbico	4116E-01016	1
Caelo	Ácido ascórbico	4565487978	1
Caelo	Ácido ascórbico	Test	1
Caesar & Loretz GmbH...	Ácido ascórbico	20003806007	1
Caesar & Loretz GmbH/Gehe	Ácido ascórbico	192143005	1
Caesar & Loretz GmbH/Gehe	Ácido ascórbico	20003806003	4
Caesar & Loretz GmbH...	Ácido ascórbico	20003806018	1
Caesar & Loretz GmbH...	Ácido ascórbico	20003806003	1
Caesar & Loretz GmbH...	Ácido ascórbico	20003806007	1
Caesar & Loretz GmbH/sana	Ácido ascórbico	19026202	1
Caesar & Loretz GmbH	Ácido ascórbico	11208606	1
Caesar & Loretz GmbH	Ácido ascórbico	12m1253	1
Caesar & Loretz GmbH	Ácido ascórbico	1542134	1
Caesar & Loretz GmbH	Ácido ascórbico	18114802	1
Caesar & Loretz GmbH	Ácido ascórbico	18127801	1
Caesar & Loretz GmbH	Ácido ascórbico	18127811	3
Caesar & Loretz GmbH	Ácido ascórbico	19026202	4
Caesar & Loretz GmbH	Ácido ascórbico	192143005	2
Caesar & Loretz GmbH	Ácido ascórbico	20001112003	4
Caesar & Loretz GmbH	Ácido ascórbico	20003806003	5
Caesar & Loretz GmbH	Ácido ascórbico	20003806005	2
Caesar & Loretz GmbH	Ácido ascórbico	20003806007	3
Caesar & Loretz GmbH	Ácido ascórbico	20003806018	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz	Ácido ascórbico	15300007	1
Caesar und Loretz	Ácido ascórbico	19026202	1
caleo	Ácido ascórbico	16345205	1
Canea Pharma/ Phönix	Ácido ascórbico	VC2014	1
Canea Pharma	Ácido ascórbico	VC1740	1
canea, gehe	Ácido ascórbico	VC1242	2
Canea/Gehe/21.10.19	Ácido ascórbico	VC1846	1
Cealo/Gehe	Ácido ascórbico	17360301	1
CSPC Weisheng	Ácido ascórbico	1211170065	1
EuRho	Ácido ascórbico	1710032-01	1
Euro OTC	Ácido ascórbico	10071418	1
Euro OTC	Ácido ascórbico	11121302	1
Euro OTC	Ácido ascórbico	12061408	1
Euro OTC	Ácido ascórbico	1607025	1
Euro OTC	Ácido ascórbico	17011404	1
Euro OTC	Ácido ascórbico	17041406	1
Euro OTC	Ácido ascórbico	1710032_01	1
Euro OTC	Ácido ascórbico	1710032-01	2
Euro OTC	Ácido ascórbico	1901044-01	1
Euro OTC	Ácido ascórbico	1909018-01	2
Euro OTC	Ácido ascórbico	191101201	1
Euro OTC	Ácido ascórbico	200202201	1
Euro OTC	Ácido ascórbico	2002022-01	10
Euro OTC	Ácido ascórbico	200202202	1
Euro OTC	Ácido ascórbico	2002022-02	6
Euro OTC	Ácido ascórbico	20020222-02	1
Euro OTC	Ácido ascórbico	2002023	1
Euro OTC	Ácido ascórbico	2002023_01	1
Euro OTC	Ácido ascórbico	2002023-01	3
Euro OTC	Ácido ascórbico	28081303	1
Euro OTC	Ácido ascórbico	DY0261921072	1
Euro OTC	Ácido ascórbico	L1202011-02	1
Euro OTC	Ácido ascórbico	L1708004	1
Euro OTC	Ácido ascórbico	L60502801	1
Fagron	Ácido ascórbico	123456	1
Fagron	Ácido ascórbico	16345205	1
Fagron	Ácido ascórbico	2002022-01	1
Fagron	Ácido ascórbico	20D14-B06-201123	1
Gatt-Koller	Ácido ascórbico	18020406	1
Gatt-Koller	Ácido ascórbico	1802406	2
Gehe/Canea	Ácido ascórbico	VC2012	1
Gehe/Gehe	Ácido ascórbico	L1505001	1
Gehe	Ácido ascórbico	16345202	1
Gehe	Ácido ascórbico	16345205	1
GEHE	Ácido ascórbico	16345205	1
GEHE	Ácido ascórbico	18127805	1
Gehe	Ácido ascórbico	20003806018	1
gehe	Ácido ascórbico	23000894001	1
Gehe	Ácido ascórbico	23000894001	1
Ge-Hh	Ácido ascórbico	192143005	1
Gesundform	Ácido ascórbico	L1110704	1
Hanse/Sana	Ácido ascórbico	233218001	1
Hänseler	Ácido ascórbico		1
Internet	Ácido ascórbico	X00162LAML	1
iuhj	Ácido ascórbico	ouhoh	1
Kehr	Ácido ascórbico	17360301	1
Kehr	Ácido ascórbico	22001801006	1
KÖGL	Ácido ascórbico	1900900	1
Ningxia	Ácido ascórbico	201114-C01-A	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Ningxia	Ácido ascórbico	201115-C01-A	1
Northeast Pharmaceut…	Ácido ascórbico	DY02622000007	1
Northeast Pharmaceut…	Ácido ascórbico	DY02622100178	2
Noweda	Ácido ascórbico	180608-C02	1
Noweda	Ácido ascórbico	1909018-01	1
Noweda	Ácido ascórbico	23000894001	1
Phoenix	Ácido ascórbico	123456789	1
Phoenix	Ácido ascórbico	18127801	2
Phoenix	Ácido ascórbico	19026202	1
Phönix	Ácido ascórbico	18127805	1
Phönix	Ácido ascórbico	20003806003	1
PHÖNIX	Ácido ascórbico	v002	1
Probe aus China	Ácido ascórbico	DY02622000011	1
Runika	Ácido ascórbico	23/10	1
Sanacorp/ Ph.Peter	Ácido ascórbico	VC2143	1
Sanacorp	Ácido ascórbico	20003806003	1
SANACORP	Ácido ascórbico	201401318	1
Sanacorp	Ácido ascórbico	2300089401	1
Shandong Luwei	Ácido ascórbico	1210111073	1
Taoasis	Ácido ascórbico	810049	1
Wep apot	Ácido ascórbico		1
wepa Apoday	Ácido ascórbico	2616110375431	1
Wepa Paulus	Ácido ascórbico	11406201	1
WEPA/Sanacorp	Ácido ascórbico	170623-C01	1
Wepa/Wepa	Ácido ascórbico	1121010319	1
wepa	Ácido ascórbico	1210142074	1
Wepa	Ácido ascórbico	170322-c01	1
Wepa	Ácido ascórbico	170322-C01	1
Wepa	Ácido ascórbico	180316-C01	1
wepa	Ácido ascórbico	180608-c02	1
wepa	Ácido ascórbico	180608-C02	1
Wepa	Ácido ascórbico	261120415	1
Wepa	Ácido ascórbico	VC2005013	1
Zentiva/Alliance Hea…	Ácido ascórbico	15300007	1

- 235 728 spectra from 1515 *Apo-Ident* customers from a total of 49 115 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido ascórbico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido ascórbico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	860	0	201 224
Type C	0	338	1	235 728

The substance/substance group *Ácido ascórbico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3023 %)
Type C	100.0000 % (> 99.9007 %)	99.7050 % (> 98.8201 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21229	21229	0,00	188,26
21317	21229	5,26	186,35
22672	22672	0,00	191,02
22680	22680	0,00	190,66
22789	22789	0,00	199,11
22918	22918	0,00	196,81
23062	23062	0,00	192,53
23288	23288	0,00	188,26
23293	23293	0,00	188,83
24936	24936	0,00	203,67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido aspártico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005413-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido aspártico; Acidum asparticum

Special notes

When selecting the *Ácido aspártico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido aspártico	2	1	0

Second-stage model

For differentiation of the substance/substance group *Ácido aspártico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido aspártico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ácido glutâmico	45,81	–
Glicina	84,89	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido aspártico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido aspártico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ácido aspártico	2108022	25775	50	20210906*
Euro OTC	Ácido aspártico	2402020	27156	30	20240322*
Euro OTC	Ácido aspártico	2402020	27156SI	20	20240322*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Ácido aspártico*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 862 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Ácido aspártico*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido aspártico	2307035	26873	40
Euro OTC	Ácido aspártico	2307035	26873SI	20

- 202 024 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ácido aspártico*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido aspártico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido aspártico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	60	0	202 024
Type C	0	0	0	236 067

The substance/substance group *Ácido aspártico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25775	25775	0,00	100,97
27156	27156	0,00	132,53

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido benzoico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20041-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido benzoico; Acidum benzoicum

Special notes

When selecting the *Ácido benzoico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido benzoico	4	2	30

Second-stage model

For differentiation of the substance/substance group *Ácido benzoico* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido benzoico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	73,11	13,34
⋮	⋮	⋮
Salicilato de sódio	>50	33,73
Cloreto de dequalínio	>50	54,06
Ácido acetilsalicílico	>50	62,25
Eosina amarela	>50	220,87
Cloridrato de oxitetraciclina	>50	328,66
Levotiroxina sódica	>50	661,20
Tanino	>50	1493,00

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido benzoico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido benzoico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido benzoico	13391310	21458	60	20131216
Caelo	Ácido benzoico	15084614	22664	40	20150318
Caelo	Ácido benzoico	15084611	23095	40	20150318
Caelo	Ácido benzoico	15084614	23096	40	1707644
Caelo	Ácido benzoico	15084614	23726	40	20150318
Caelo	Ácido benzoico	23001052	26693	40	20230601*
Caelo	Ácido benzoico	23001052	26693SI	20	20230601*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Ácido benzoico*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 682 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Ácido benzoico*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido benzoico	162701	24027	40
Caelo	Ácido benzoico	190752	24532	40

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 99 spectra from 71 *Apo-Ident* customers from 32 batches from the substance/substance group *Ácido benzoico*.

- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
ACM	Ácido benzoico	KNC0396J17	1
ACM	Ácido benzoico	KNC0558J15	1
Anza	Ácido benzoico	16001702	1
Anzag	Ácido benzoico	16001708	1
Caelo	Ácido benzoico	10156104	1
Caelo	Ácido benzoico	13074605	3
Caelo	Ácido benzoico	13074610	4
Caelo	Ácido benzoico	1339120	1
Caelo	Ácido benzoico	13391310	1
Caelo	Ácido benzoico	13391314	1
Caelo	Ácido benzoico	13391320	1
Caelo	Ácido benzoico	15084603	3
Caelo	Ácido benzoico	15084607	4
Caelo	Ácido benzoico	15084614	2
Caelo	Ácido benzoico	15084701	1
Caelo	Ácido benzoico	16001702	2
Caelo	Ácido benzoico	16001708	2
Caelo	Ácido benzoico	16001714	7
Caelo	Ácido benzoico	17327003	2
Caelo	Ácido benzoico	17327004	1
Caelo	Ácido benzoico	17327006	1
Caelo	Ácido benzoico	17327009	2
Caelo	Ácido benzoico	1732701	1
Caelo	Ácido benzoico	17327013	6
Caelo	Ácido benzoico	17327101	10
Caelo	Ácido benzoico	190752005	1
Caelo	Ácido benzoico	190752007	6
Caelo	Ácido benzoico	20003734002	4
Caelo	Ácido benzoico	20003734004	1
Caelo	Ácido benzoico	20003734006	2
Caesar & Loretz GmbH…	Ácido benzoico	17327013	2
Caesar & Loretz GmbH/Gehe	Ácido benzoico	20003734004	1
Caesar & Loretz GmbH	Ácido benzoico	17327003	2
Caesar & Loretz GmbH	Ácido benzoico	17327006	2
Caesar & Loretz GmbH	Ácido benzoico	17327009	1
Caesar & Loretz GmbH	Ácido benzoico	17327013	1
Caesar & Loretz GmbH	Ácido benzoico	190752007	1
Caesar & Loretz GmbH	Ácido benzoico	20003734004	1
Caesar & Loretz GmbH	Ácido benzoico	20003734006	1
Caesar & Loretz GmbH	Ácido benzoico	20003734013	1
Caleo/Phoenix	Ácido benzoico	15084607	1
Cealo, GEHE	Ácido benzoico	20003734002	1
Cealo	Ácido benzoico	13391314	1
Fresenius	Ácido benzoico	80715102	1
Gatt-Koller / Phoenix	Ácido benzoico	2992/07131314	2
Gehe	Ácido benzoico	22001605009	1
Phönix	Ácido benzoico	13074605	2
Phönix	Ácido benzoico	16001714	1
Phönix	Ácido benzoico	17327003	1
Sanacorp	Ácido benzoico	16001714	1

- 235 968 spectra from 1515 *Apo-Ident* customers from a total of 49 226 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ácido benzoico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido benzoico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	80	0	202 004
Type C	0	99	0	235 968

The substance/substance group *Ácido benzoico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.9394 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21458	23096	17,95	116,71
22664	26693	16,00	116,50
23095	26693	14,86	116,10
23096	23096	0,00	119,78
23726	23096	8,30	119,51
26693	26693	0,00	120,91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido bórico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20182-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido bórico; Acidum boricum

Special notes

When selecting the *Ácido bórico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido bórico	6	5	44

Second-stage model

For differentiation of the substance/substance group *Ácido bórico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido bórico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	93,46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido bórico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido bórico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido bórico	14133119	21804	60	20140509
Caelo	Ácido bórico	15425112	22964	40	20160104
Caelo	Ácido bórico	170613	23286	40	20170316*
Caelo	Ácido bórico	193010	25210	40	20200113*
Fagron	Ácido bórico	13I04-N06	21228	40	20130920
Fagron	Ácido bórico	15L09-B07-322988	23746	40	20151222

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 260 spectra of 6 reference samples from the substance/substance group *Ácido bórico*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Ácido bórico*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido bórico	15242903	22965	40
Caelo	Ácido bórico	191943	24741	40
Caelo	Ácido bórico	21001289	25698	50
Caelo	Ácido bórico	21000784	25701	50
Caelo	Ácido bórico	24001235	27258	40
Caelo	Ácido bórico	24001235	27258SI	20

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 81 spectra from 57 *Apo-Ident* customers from 49 batches from the substance/substance group *Ácido bórico*.

- Among them are spectra of independent samples from 44 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Ácido bórico	10227913	1
Caelo	Ácido bórico	11D13-N08	1
Caelo	Ácido bórico	12238901	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido bórico	12260502	1
Caelo	Ácido bórico	14095202	1
Caelo	Ácido bórico	14133113	2
Caelo	Ácido bórico	14133119	1
Caelo	Ácido bórico	15095103	2
Caelo	Ácido bórico	15158901	1
Caelo	Ácido bórico	15158903	1
Caelo	Ácido bórico	15242906	1
Caelo	Ácido bórico	15242909	1
Caelo	Ácido bórico	15425101	5
Caelo	Ácido bórico	15425108	2
Caelo	Ácido bórico	15425112	2
Caelo	Ácido bórico	15425114	2
Caelo	Ácido bórico	15425118	3
Caelo	Ácido bórico	16291001	1
Caelo	Ácido bórico	17327901	4
Caelo	Ácido bórico	17327907	5
Caelo	Ácido bórico	17327912	2
Caelo	Ácido bórico	17327917	3
Caelo	Ácido bórico	193010003	1
Caelo	Ácido bórico	19301003	1
Caelo	Ácido bórico	20000508002	2
Caelo	Ácido bórico	20000508005	2
Caelo	Ácido bórico	200041/5001	1
Caelo	Ácido bórico	20004175001	1
Caelo	Ácido bórico	21000784001	1
Caelo	Ácido bórico	5425114	1
Caelo	Ácido bórico	80303AB	1
Caelo	Ácido bórico	9324021	1
Caelo	Ácido bórico	9324036	1
Caelo	Ácido bórico	9324043	1
Caesar & Loretz GmbH…	Ácido bórico	20000508002	1
Caesar & Loretz GmbH/Kehr	Ácido bórico	17327916	1
Caesar & Loretz GmbH	Ácido bórico	17327912	2
Caesar & Loretz GmbH	Ácido bórico	17327916	1
Caesar & Loretz GmbH	Ácido bórico	19194301	1
Caesar & Loretz GmbH	Ácido bórico	20000508002	2
Caesar & Loretz GmbH	Ácido bórico	20004175001	1
E Plus	Ácido bórico	15425108	1
Fagron	Ácido bórico	11d13-n08	1
Fagron	Ácido bórico	11I26-n05	1
Fagron	Ácido bórico	12f01-n08	1
Fagron	Ácido bórico	12G04-N10	1
Fagron	Ácido bórico	13A21-N06	1
Fagron	Ácido bórico	13I04-N06	2
Fagron	Ácido bórico	14133101	1
Fagron	Ácido bórico	14B07-B02-295752	1
Fagron	Ácido bórico	9082012B	1
Gatt-Koller	Ácido bórico	1803542	1
Labor	Ácido bórico	159095	1
Nachprüfung	Ácido bórico		1
Sanacorp	Ácido bórico	1/AKD3	1

- 235 986 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ácido bórico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido bórico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	240	0	201 844
Type C	0	81	0	235 986

The substance/substance group *Ácido bórico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.5926 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21228	25210	10,83	167,63
21804	25210	3,85	165,22
22964	23286	15,58	179,31
23286	23286	0,00	199,91
23746	25210	9,94	169,42
25210	25210	0,00	171,74

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido cítrico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20019-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido cítrico; Acidum citricum

Special notes

When selecting the *Ácido cítrico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido cítrico	8	25	647

Second-stage model

For differentiation of the substance/substance group *Ácido cítrico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido cítrico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citrato monobásico de magnésio, hid…	92,94	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido cítrico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido cítrico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido cítrico	11380204	20682	40	20120127
Caelo	Ácido cítrico	12043112	20683	40	20120229
Caelo	Ácido cítrico	13396502	21455	60	20140110
Caelo	Ácido cítrico	13243213	21487	40	20130821
Caelo	Ácido cítrico	160386	22463	60	20160315*
Caelo	Ácido cítrico	22002250	26350	40	20220912*
Caelo	Ácido cítrico	22002250	26350SI	20	20220912*
Fagron	Ácido cítrico	12F18-N03	20706	40	20120628
Fagron	Ácido cítrico	13G24-N13	20913	40	20130827

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 9 reference samples from the substance/substance group *Ácido cítrico*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 582 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1170 spectra of 31 reference samples from the substance/substance group *Ácido cítrico*.

- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido cítrico	160387	22478	60
Caelo	Ácido cítrico	162086	22620	40
Caelo	Ácido cítrico	162154	22622	40
Caelo	Ácido cítrico	171627	23303	40
Caelo	Ácido cítrico	171626	23421	40
Caelo	Ácido cítrico	180976	24034	40
Caelo	Ácido cítrico	181292	24232	40
Caelo	Ácido cítrico	183121	24366	40
Caelo	Ácido cítrico	183071	24367	40
Caelo	Ácido cítrico	192036	24740	40
Caelo	Ácido cítrico	192073	24744	40
Caelo	Ácido cítrico	21000543	25631	40
Caelo	Ácido cítrico	21000544	25635	40
Caelo	Ácido cítrico	21002657	25855	50
Caelo	Ácido cítrico	22000645	26122	40
Caelo	Ácido cítrico	22002309	26358	40
Caelo	Ácido cítrico	23002104	26946	40
Caelo	Ácido cítrico	23002107	26955	40
Caelo	Ácido cítrico	24001159	27253	40
Euro OTC	Ácido cítrico	2112002	25947	40
Euro OTC	Ácido cítrico	2301021	26510	40
Euro OTC	Ácido cítrico	2310005	27007	40
Euro OTC	Ácido cítrico	2407008	27457	40
Fagron	Ácido cítrico	21F11-B04-213849	26146	40
Fagron	Ácido cítrico	23C01-B01-228324	26828	30
Caelo	Ácido cítrico	171626	23648	40
Caelo	Ácido cítrico	171627	23677	40
Caelo	Ácido cítrico	22000645	26122SI	20
Caelo	Ácido cítrico	22002309	26358SI	20

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido cítrico	2112002	25947SI	10
Fagron	Ácido cítrico	21F11-B04-213849	26146SI	20

- 200 914 spectra from a total of 4020 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4343 spectra from 1217 *Apo-Ident* customers from 666 batches from the substance/substance group *Ácido cítrico*.
- Among them are spectra of independent samples from 642 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido cítrico	12345	1
	Ácido cítrico	13K18-B34-291523	1
	Ácido cítrico	2000645001	1
	Ácido cítrico	21000543008	1
	Ácido cítrico	21000543010	1
	Ácido cítrico	21000544002	1
	Ácido cítrico	21002657002	2
	Ácido cítrico	21002657003	1
	Ácido cítrico	21002657006	1
	Ácido cítrico	21002657007	1
	Ácido cítrico	21002657012	4
	Ácido cítrico	21002657015	13
	Ácido cítrico	21002657016	1
	Ácido cítrico	21002657017	7
	Ácido cítrico	2112002-03	2
	Ácido cítrico	220000645004	1
	Ácido cítrico	22000645001	2
	Ácido cítrico	22000645005	1
	Ácido cítrico	22000645009	6
	Ácido cítrico	22000645011	5
	Ácido cítrico	220021564	1
	Ácido cítrico	22002250001	5
	Ácido cítrico	22002250004	2
	Ácido cítrico	22002309001	7
	Ácido cítrico	22002309004	10
	Ácido cítrico	22H11-B02-227794	1
	Ácido cítrico	22I05-B07-222923	1
	Ácido cítrico	22I05-B07-225242	1
	Ácido cítrico	23003597001	1
	Ácido cítrico	2301021-01	1
	Ácido cítrico	23568	1
	Ácido cítrico	6491041	1
092522438	Ácido cítrico	22000645001	2
12.12.2016 Phoenix 4,59EUR	Ácido cítrico	15088008	1
A.H. 08.06.13 ek: 6,92EUR	Ácido cítrico	13050604	1
AEP	Ácido cítrico	22002309004	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Ácido cítrico	13050607	1
AHD	Ácido cítrico	13396502	1
AHD	Ácido cítrico	15063218	1
AHD	Ácido cítrico	16208614	1
AHD	Ácido cítrico	17329511	2
AHD	Ácido cítrico	20000886003	1
AHD	Ácido cítrico	21000543008	1
AHD	Ácido cítrico	21002657003	1
AHD	Ácido cítrico	21002657015	2
AHD	Ácido cítrico	22000645001	1
ALH	Ácido cítrico	L1508013-01	1
Alliance Health 03.0...	Ácido cítrico	13K18-B34	1
Alliance Healthcare	Ácido cítrico	12043123	1
ALLIANCE HEALTHCARE	Ácido cítrico	19003185	1
Alliance Healthcare	Ácido cítrico	21000543008	1
Anzag	Ácido cítrico	10049712	1
Anzag	Ácido cítrico	10049713	1
anzag	Ácido cítrico	13175409	1
Anzag	Ácido cítrico	192073009	2
Anzag	Ácido cítrico	21002657017	1
Anzag	Ácido cítrico	6494061	1
apomix	Ácido cítrico	16208612	2
Apotheke	Ácido cítrico	21000543005	1
Audor Pharma	Ácido cítrico	PA201	1
Beyvers	Ácido cítrico	16038606	1
Bombastus	Ácido cítrico	12250004-3-0	1
Bombastus	Ácido cítrico	13396502	1
Bombastus	Ácido cítrico	17162601	2
Bombastus	Ácido cítrico	17162602	1
Bombastus	Ácido cítrico	18097060	1
Bombastus	Ácido cítrico	20002872	1
Bombastus	Ácido cítrico	21004820	1
Bombastus	Ácido cítrico	272757	2
Caelo	Ácido cítrico		8
Caelo	Ácido cítrico	10049716	1
Caelo	Ácido cítrico	1015U-01024	1
Caelo	Ácido cítrico	10182420	1
Caelo	Ácido cítrico	1044905	1
Caelo	Ácido cítrico	1072015B	1
Caelo	Ácido cítrico	11066806	1
Caelo	Ácido cítrico	11159801	2
Caelo	Ácido cítrico	11159817	1
Caelo	Ácido cítrico	11159821	1
Caelo	Ácido cítrico	11159824	1
Caelo	Ácido cítrico	11178303	5
Caelo	Ácido cítrico	11189817	1
Caelo	Ácido cítrico	11380204	5
Caelo	Ácido cítrico	11380208	1
Caelo	Ácido cítrico	11380213	1
Caelo	Ácido cítrico	11380215	3
Caelo	Ácido cítrico	11380217	2
Caelo	Ácido cítrico	1150817/16208614	1
Caelo	Ácido cítrico	1155609	2
Caelo	Ácido cítrico	1172673	1
Caelo	Ácido cítrico	1175409	2
Caelo	Ácido cítrico	1181765	2
Caelo	Ácido cítrico	11C24-N02	1
Caelo	Ácido cítrico	11C24-N03	1
Caelo	Ácido cítrico	11K07-N01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	11K11-N02	1
Caelo	Ácido cítrico	12043105	2
Caelo	Ácido cítrico	12043110	4
Caelo	Ácido cítrico	12043112	3
Caelo	Ácido cítrico	12043113	3
Caelo	Ácido cítrico	12043118	3
Caelo	Ácido cítrico	12043119	1
Caelo	Ácido cítrico	12043120	5
Caelo	Ácido cítrico	12043123	6
Caelo	Ácido cítrico	12043124	3
Caelo	Ácido cítrico	12156801	2
Caelo	Ácido cítrico	12156803	8
Caelo	Ácido cítrico	12156804	3
Caelo	Ácido cítrico	12156811	11
Caelo	Ácido cítrico	12156812	4
Caelo	Ácido cítrico	12156818	1
Caelo	Ácido cítrico	12156822	2
Caelo	Ácido cítrico	12156823	4
Caelo	Ácido cítrico	12156824	5
Caelo	Ácido cítrico	12156827	1
Caelo	Ácido cítrico	12156830	1
Caelo	Ácido cítrico	12156832	7
Caelo	Ácido cítrico	121568704	1
Caelo	Ácido cítrico	12175708	3
Caelo	Ácido cítrico	12175711	1
Caelo	Ácido cítrico	12175716	2
Caelo	Ácido cítrico	12175717	1
Caelo	Ácido cítrico	12175718	1
Caelo	Ácido cítrico	1218A-01024	2
Caelo	Ácido cítrico	1230616	1
Caelo	Ácido cítrico	12345	1
Caelo	Ácido cítrico	12353613	1
Caelo	Ácido cítrico	125356	1
Caelo	Ácido cítrico	12B01-N01	5
Caelo	Ácido cítrico	13011801	1
Caelo	Ácido cítrico	13031502	1
Caelo	Ácido cítrico	13050601	9
Caelo	Ácido cítrico	13050604	13
Caelo	Ácido cítrico	13050606	2
Caelo	Ácido cítrico	13050607	9
Caelo	Ácido cítrico	13050610	6
Caelo	Ácido cítrico	13050611	6
Caelo	Ácido cítrico	13050613	18
Caelo	Ácido cítrico	13050614	7
Caelo	Ácido cítrico	13050617	12
Caelo	Ácido cítrico	13050618	3
Caelo	Ácido cítrico	13050621	2
Caelo	Ácido cítrico	13050622	7
Caelo	Ácido cítrico	13050623	2
Caelo	Ácido cítrico	13050623-3376319052	1
Caelo	Ácido cítrico	13050624	1
Caelo	Ácido cítrico	1305601	1
Caelo	Ácido cítrico	13061502	1
Caelo	Ácido cítrico	1306911	1
Caelo	Ácido cítrico	130-7612	1
Caelo	Ácido cítrico	13157404	1
Caelo	Ácido cítrico	13175402	3
Caelo	Ácido cítrico	13175403	14
Caelo	Ácido cítrico	13175404	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	13175405	5
Caelo	Ácido cítrico	13175406	3
Caelo	Ácido cítrico	13175409	20
Caelo	Ácido cítrico	13175410	4
Caelo	Ácido cítrico	13175411	10
Caelo	Ácido cítrico	13175414	2
Caelo	Ácido cítrico	13175426	4
Caelo	Ácido cítrico	13243005	1
Caelo	Ácido cítrico	13243201	17
Caelo	Ácido cítrico	13243202	10
Caelo	Ácido cítrico	13243208	2
Caelo	Ácido cítrico	13243210	10
Caelo	Ácido cítrico	13243213	21
Caelo	Ácido cítrico	13243214	15
Caelo	Ácido cítrico	13243216	11
Caelo	Ácido cítrico	13243217	6
Caelo	Ácido cítrico	13243218	9
Caelo	Ácido cítrico	13243219	4
Caelo	Ácido cítrico	13243220	2
Caelo	Ácido cítrico	13243221	8
Caelo	Ácido cítrico	13243222	1
Caelo	Ácido cítrico	13243224	2
Caelo	Ácido cítrico	13243225	4
Caelo	Ácido cítrico	13243229	2
Caelo	Ácido cítrico	133243218	1
Caelo	Ácido cítrico	13396502	3
Caelo	Ácido cítrico	13396504	3
Caelo	Ácido cítrico	13396505	3
Caelo	Ácido cítrico	13396506	1
Caelo	Ácido cítrico	13396515	2
Caelo	Ácido cítrico	1380208	1
Caelo	Ácido cítrico	1396505	1
Caelo	Ácido cítrico	13A04-N04	4
Caelo	Ácido cítrico	13D29-N02	1
Caelo	Ácido cítrico	13G24-N13	4
Caelo	Ácido cítrico	13K18-B34	1
Caelo	Ácido cítrico	13K18-B34-288371TEST	1
Caelo	Ácido cítrico	13K18-B34-288372	1
Caelo	Ácido cítrico	13K18-B34-291520	1
Caelo	Ácido cítrico	13K18-B34-291522	1
Caelo	Ácido cítrico	13K18-B34-291523	2
Caelo	Ácido cítrico	14041506	1
Caelo	Ácido cítrico	14071501	1
Caelo	Ácido cítrico	14162701	1
Caelo	Ácido cítrico	14186301	23
Caelo	Ácido cítrico	14186302	14
Caelo	Ácido cítrico	14186312	16
Caelo	Ácido cítrico	14186313	11
Caelo	Ácido cítrico	14186314	4
Caelo	Ácido cítrico	1418E-01024	1
Caelo	Ácido cítrico	14E06-B07	1
Caelo	Ácido cítrico	14G04-B09	1
Caelo	Ácido cítrico	14G04-B09-293874	2
Caelo	Ácido cítrico	14G04-B09-293876	4
Caelo	Ácido cítrico	14G04B09293877	1
Caelo	Ácido cítrico	14K05-B04-302815	1
Caelo	Ácido cítrico	1501-B06-324348	1
Caelo	Ácido cítrico	15044901	9
Caelo	Ácido cítrico	15044902	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	15044903	5
Caelo	Ácido cítrico	15044904	10
Caelo	Ácido cítrico	15044905	10
Caelo	Ácido cítrico	15063003	26
Caelo	Ácido cítrico	15063003-20160615Ma1	1
Caelo	Ácido cítrico	15063006	5
Caelo	Ácido cítrico	150632	1
Caelo	Ácido cítrico	15063202	1
Caelo	Ácido cítrico	15063203	15
Caelo	Ácido cítrico	15063204	14
Caelo	Ácido cítrico	15063205	3
Caelo	Ácido cítrico	15063206	23
Caelo	Ácido cítrico	15063211	5
Caelo	Ácido cítrico	15063213	27
Caelo	Ácido cítrico	15063214	9
Caelo	Ácido cítrico	15063217	12
Caelo	Ácido cítrico	15063218	11
Caelo	Ácido cítrico	15087510	1
Caelo	Ácido cítrico	15087902	3
Caelo	Ácido cítrico	15087903	19
Caelo	Ácido cítrico	15087904	1
Caelo	Ácido cítrico	15088008	2
Caelo	Ácido cítrico	15088016	4
Caelo	Ácido cítrico	15088017	2
Caelo	Ácido cítrico	15091401	1
Caelo	Ácido cítrico	15124202	1
Caelo	Ácido cítrico	15124301	10
Caelo	Ácido cítrico	15124303	1
Caelo	Ácido cítrico	1516Q-01024	1
Caelo	Ácido cítrico	15185320	1
Caelo	Ácido cítrico	15214301	1
Caelo	Ácido cítrico	15G16-B01-330449	2
Caelo	Ácido cítrico	15G16-B01-330450	1
Caelo	Ácido cítrico	16004701	21
Caelo	Ácido cítrico	16004702	28
Caelo	Ácido cítrico	16004705	4
Caelo	Ácido cítrico	16004706	23
Caelo	Ácido cítrico	16038602	3
Caelo	Ácido cítrico	16038603	5
Caelo	Ácido cítrico	16038604	9
Caelo	Ácido cítrico	16038606	24
Caelo	Ácido cítrico	16038607	7
Caelo	Ácido cítrico	16038608	14
Caelo	Ácido cítrico	16038613	10
Caelo	Ácido cítrico	16038614	5
Caelo	Ácido cítrico	16038617	2
Caelo	Ácido cítrico	16038621	19
Caelo	Ácido cítrico	16038622	9
Caelo	Ácido cítrico	16038701	5
Caelo	Ácido cítrico	16038704	12
Caelo	Ácido cítrico	16038707	11
Caelo	Ácido cítrico	16038708	9
Caelo	Ácido cítrico	16038709	6
Caelo	Ácido cítrico	16038710	3
Caelo	Ácido cítrico	16038712	7
Caelo	Ácido cítrico	16038713	1
Caelo	Ácido cítrico	160607AC	1
Caelo	Ácido cítrico	160614	1
Caelo	Ácido cítrico	1606141	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	160808/3	1
Caelo	Ácido cítrico	16088607	1
Caelo	Ácido cítrico	1620610	1
Caelo	Ácido cítrico	16206813	1
Caelo	Ácido cítrico	16208605	16
Caelo	Ácido cítrico	162086055525	1
Caelo	Ácido cítrico	16208606	31
Caelo	Ácido cítrico	16208607	33
Caelo	Ácido cítrico	16208608	6
Caelo	Ácido cítrico	16208610	14
Caelo	Ácido cítrico	16208612	25
Caelo	Ácido cítrico	16208613	13
Caelo	Ácido cítrico	16208614	56
Caelo	Ácido cítrico	16208615	3
Caelo	Ácido cítrico	162088606	1
Caelo	Ácido cítrico	162154	1
Caelo	Ácido cítrico	16215403	3
Caelo	Ácido cítrico	16215405	6
Caelo	Ácido cítrico	16215408	6
Caelo	Ácido cítrico	16215409	10
Caelo	Ácido cítrico	170607C/16208605	1
Caelo	Ácido cítrico	17071301	1
Caelo	Ácido cítrico	17161601	1
Caelo	Ácido cítrico	17162601	34
Caelo	Ácido cítrico	17162602	29
Caelo	Ácido cítrico	17162603	9
Caelo	Ácido cítrico	17162604	3
Caelo	Ácido cítrico	1716262601	1
Caelo	Ácido cítrico	17162701	32
Caelo	Ácido cítrico	17162702	12
Caelo	Ácido cítrico	17162706	1
Caelo	Ácido cítrico	1716271	1
Caelo	Ácido cítrico	171652601	1
Caelo	Ácido cítrico	173295002	1
Caelo	Ácido cítrico	17329502	20
Caelo	Ácido cítrico	17329503	8
Caelo	Ácido cítrico	17329504	2
Caelo	Ácido cítrico	17329511	10
Caelo	Ácido cítrico	17329512	3
Caelo	Ácido cítrico	17329513	3
Caelo	Ácido cítrico	177162601	1
Caelo	Ácido cítrico	17E15-B04-335435	1
Caelo	Ácido cítrico	17E15-B04-339371	1
Caelo	Ácido cítrico	180257004	1
Caelo	Ácido cítrico	18025701	48
Caelo	Ácido cítrico	18025702	55
Caelo	Ácido cítrico	18025704	22
Caelo	Ácido cítrico	180257045617	1
Caelo	Ácido cítrico	18025801	30
Caelo	Ácido cítrico	18025802	6
Caelo	Ácido cítrico	180297609	1
Caelo	Ácido cítrico	18091409	1
Caelo	Ácido cítrico	18097202	1
Caelo	Ácido cítrico	18097601	48
Caelo	Ácido cítrico	18097602	15
Caelo	Ácido cítrico	18097603	25
Caelo	Ácido cítrico	18097604	1
Caelo	Ácido cítrico	18097606	19
Caelo	Ácido cítrico	18097607	21

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	18097609	33
Caelo	Ácido cítrico	18097610	1
Caelo	Ácido cítrico	18097611	24
Caelo	Ácido cítrico	18097615	1
Caelo	Ácido cítrico	18111704	1
Caelo	Ácido cítrico	1812104	1
Caelo	Ácido cítrico	1812905	2
Caelo	Ácido cítrico	18129204	3
Caelo	Ácido cítrico	18129205	37
Caelo	Ácido cítrico	18129206	4
Caelo	Ácido cítrico	18129207	5
Caelo	Ácido cítrico	183006905	1
Caelo	Ácido cítrico	18304909	1
Caelo	Ácido cítrico	18306902	34
Caelo	Ácido cítrico	18306903	27
Caelo	Ácido cítrico	18306905	50
Caelo	Ácido cítrico	18306905P-190531-4	1
Caelo	Ácido cítrico	18306906	50
Caelo	Ácido cítrico	18306908	9
Caelo	Ácido cítrico	18306909	39
Caelo	Ácido cítrico	18306911	65
Caelo	Ácido cítrico	18306913	2
Caelo	Ácido cítrico	183069606	1
Caelo	Ácido cítrico	18306999	1
Caelo	Ácido cítrico	18307101	2
Caelo	Ácido cítrico	18307102	12
Caelo	Ácido cítrico	18307104	17
Caelo	Ácido cítrico	1831209	1
Caelo	Ácido cítrico	18312102	3
Caelo	Ácido cítrico	18312103	2
Caelo	Ácido cítrico	18312104	18
Caelo	Ácido cítrico	18312107	1
Caelo	Ácido cítrico	18312109	10
Caelo	Ácido cítrico	1836911	1
Caelo	Ácido cítrico	18F25-B02	1
Caelo	Ácido cítrico	18F25-B02-351453	1
Caelo	Ácido cítrico	18F25-B02-351454	1
Caelo	Ácido cítrico	19041304	1
Caelo	Ácido cítrico	19041305	1
Caelo	Ácido cítrico	1917A-01024	1
Caelo	Ácido cítrico	192036002	5
Caelo	Ácido cítrico	192036003	27
Caelo	Ácido cítrico	1920366003	1
Caelo	Ácido cítrico	192037005	1
Caelo	Ácido cítrico	192073002	32
Caelo	Ácido cítrico	192073003	18
Caelo	Ácido cítrico	192073003P-200602-1	1
Caelo	Ácido cítrico	192073004	43
Caelo	Ácido cítrico	192073005	33
Caelo	Ácido cítrico	192073005P-200507-3	1
Caelo	Ácido cítrico	192073005P-200609-5	1
Caelo	Ácido cítrico	192073009	27
Caelo	Ácido cítrico	192073010	2
Caelo	Ácido cítrico	19H23-B07-194438	1
Caelo	Ácido cítrico	200000886003	1
Caelo	Ácido cítrico	200003515014	1
Caelo	Ácido cítrico	200008860003	1
Caelo	Ácido cítrico	20000886001	2
Caelo	Ácido cítrico	20000886002	44

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	20000886003	65
Caelo	Ácido cítrico	20000886006	1
Caelo	Ácido cítrico	20000886007	30
Caelo	Ácido cítrico	20000886009	39
Caelo	Ácido cítrico	20000886012	1
Caelo	Ácido cítrico	20000889002	1
Caelo	Ácido cítrico	20003515003	16
Caelo	Ácido cítrico	20003515007	1
Caelo	Ácido cítrico	20003515008	4
Caelo	Ácido cítrico	20003515009	1
Caelo	Ácido cítrico	20003515010	4
Caelo	Ácido cítrico	20003515013	1
Caelo	Ácido cítrico	20003515014	8
Caelo	Ácido cítrico	2000886007	2
Caelo	Ácido cítrico	20060912-3	1
Caelo	Ácido cítrico	20151112-1	1
Caelo	Ácido cítrico	2017-04-18AVLu	1
Caelo	Ácido cítrico	20170728/Ma1	1
Caelo	Ácido cítrico	2019Q-01024	1
Caelo	Ácido cítrico	2051703	1
Caelo	Ácido cítrico	2071303	1
Caelo	Ácido cítrico	20F19-B01-201169	1
Caelo	Ácido cítrico	210000200004	1
Caelo	Ácido cítrico	21000020004	2
Caelo	Ácido cítrico	210000543005	1
Caelo	Ácido cítrico	210000543011	1
Caelo	Ácido cítrico	21000211004	1
Caelo	Ácido cítrico	210002657003	1
Caelo	Ácido cítrico	2100054002	1
Caelo	Ácido cítrico	21000542008	1
Caelo	Ácido cítrico	21000543001	1
Caelo	Ácido cítrico	21000543002	8
Caelo	Ácido cítrico	21000543003	20
Caelo	Ácido cítrico	21000543004	1
Caelo	Ácido cítrico	21000543005	13
Caelo	Ácido cítrico	21000543006	3
Caelo	Ácido cítrico	21000543008	21
Caelo	Ácido cítrico	21000543010	5
Caelo	Ácido cítrico	21000543011	6
Caelo	Ácido cítrico	21000544001	11
Caelo	Ácido cítrico	21000544002	58
Caelo	Ácido cítrico	21000544003	2
Caelo	Ácido cítrico	21000544004	10
Caelo	Ácido cítrico	21000544006	8
Caelo	Ácido cítrico	2100054401	1
Caelo	Ácido cítrico	2100054402	1
Caelo	Ácido cítrico	2100054404	1
Caelo	Ácido cítrico	210005543003	1
Caelo	Ácido cítrico	21002657001	9
Caelo	Ácido cítrico	21002657002	10
Caelo	Ácido cítrico	21002657003	32
Caelo	Ácido cítrico	21002657004	1
Caelo	Ácido cítrico	21002657006	9
Caelo	Ácido cítrico	21002657012	5
Caelo	Ácido cítrico	21002657015	12
Caelo	Ácido cítrico	21002657016	4
Caelo	Ácido cítrico	2100543006	1
Caelo	Ácido cítrico	2100544002	1
Caelo	Ácido cítrico	2100544004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico	21531	1
Caelo	Ácido cítrico	22000645001	8
Caelo	Ácido cítrico	22000645004	2
Caelo	Ácido cítrico	22000645005	2
Caelo	Ácido cítrico	22000645008	1
Caelo	Ácido cítrico	22002309004	1
Caelo	Ácido cítrico	2317M-01024	1
Caelo	Ácido cítrico	2317Q-01024	1
Caelo	Ácido cítrico	24021502	1
Caelo	Ácido cítrico	26051803	1
Caelo	Ácido cítrico	26071701	1
Caelo	Ácido cítrico	26111301	1
Caelo	Ácido cítrico	2617Q-01024	1
Caelo	Ácido cítrico	27091303	1
Caelo	Ácido cítrico	2716A-01024	1
Caelo	Ácido cítrico	2789	1
Caelo	Ácido cítrico	28021405	1
Caelo	Ácido cítrico	28051401	1
Caelo	Ácido cítrico	3091701	1
Caelo	Ácido cítrico	3275	1
Caelo	Ácido cítrico	4918Q-01024	1
Caelo	Ácido cítrico	501170606	1
Caelo	Ácido cítrico	5041802	1
Caelo	Ácido cítrico	5315I-01024	1
Caelo	Ácido cítrico	59(20000886009)	1
Caelo	Ácido cítrico	6071713	1
Caelo	Ácido cítrico	6498011	2
Caelo	Ácido cítrico	713I-01024	1
Caelo	Ácido cítrico	7808	2
Caelo	Ácido cítrico	8031702	1
Caelo	Ácido cítrico	8306911	1
Caelo	Ácido cítrico	886007	1
Caelo	Ácido cítrico	9158408	1
Caelo	Ácido cítrico	9199105	1
Caelo	Ácido cítrico	9494185	1
Caelo	Ácido cítrico	A-040513-1	1
Caelo	Ácido cítrico	AP220721-01	1
Caelo	Ácido cítrico	jjjjjj	1
Caelo	Ácido cítrico	L130404202	1
Caelo	Ácido cítrico	L1508013-01	1
Caelo	Ácido cítrico	L1609021-01	3
Caelo	Ácido cítrico	L1805017-03	2
Caelo	Ácido cítrico	P-12061921/18097611	1
Caelo	Ácido cítrico	P-12081922/18312102	1
Caelo	Ácido cítrico	P170612AC06/19	1
Caelo	Ácido cítrico	xxxx	1
Caelo	Ácido cítrico	xxxxxx	1
Caeolo/Gehe	Ácido cítrico	15044903	3
Caesar & Lorenz GmbH	Ácido cítrico	16004706	1
Caesar & Lorenz	Ácido cítrico	21002657003	1
Caesar & Loretz /Sanacorp	Ácido cítrico	20000886002	1
Caesar & Loretz GmbH...	Ácido cítrico	22002309004	1
Caesar & Loretz GmbH...	Ácido cítrico	16208614	1
Caesar & Loretz GmbH...	Ácido cítrico	15063203	1
Caesar & Loretz GmbH...	Ácido cítrico	192073002	1
Caesar & Loretz GmbH...	Ácido cítrico	21000543003	1
Caesar & Loretz GmbH...	Ácido cítrico	18306906	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886009	1
Caesar & Loretz GmbH...	Ácido cítrico	18025702	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Ácido cítrico	18097609	2
Caesar & Loretz GmbH...	Ácido cítrico	18097611	1
Caesar & Loretz GmbH...	Ácido cítrico	192073003	1
Caesar & Loretz GmbH...	Ácido cítrico	192073005	1
Caesar & Loretz GmbH...	Ácido cítrico	192073009	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544006	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544001	1
Caesar & Loretz GmbH...	Ácido cítrico	18306905	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH /G	Ácido cítrico	18306911	1
Caesar & Loretz GmbH/ AEP	Ácido cítrico	192073003	1
Caesar & Loretz GmbH...	Ácido cítrico	17162712	1
Caesar & Loretz GmbH...	Ácido cítrico	18306909	1
Caesar & Loretz GmbH...	Ácido cítrico	192073009	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886003	1
Caesar & Loretz GmbH/AEP	Ácido cítrico	192073005	1
Caesar & Loretz GmbH/AEP	Ácido cítrico	21002657001	1
Caesar & Loretz GmbH/AHD	Ácido cítrico	18306906	1
Caesar & Loretz GmbH/AHD	Ácido cítrico	192073005	2
Caesar & Loretz GmbH/AHD	Ácido cítrico	20000886003	1
Caesar & Loretz GmbH/AHD	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH...	Ácido cítrico	21000543011	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544001	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886003	1
Caesar & Loretz GmbH/E	Ácido cítrico	21000543003	1
Caesar & Loretz GmbH...	Ácido cítrico	18306902	1
Caesar & Loretz GmbH...	Ácido cítrico	192073009	1
Caesar & Loretz GmbH...	Ácido cítrico	21000543010	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	18129211	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	18306905	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	18306911	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	18307104	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	18312107	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	192073005	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	192073009	2
Caesar & Loretz GmbH/Gehe	Ácido cítrico	20000886007	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	20000886009	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico	20003515003	1
Caesar & Loretz GmbH/GEHE	Ácido cítrico	20003515004	1
Caesar & Loretz GmbH/GEHE	Ácido cítrico	21000544001	1
Caesar & Loretz GmbH...	Ácido cítrico	21002657006	1
Caesar & Loretz GmbH...	Ácido cítrico	19073004	1
Caesar & Loretz GmbH...	Ácido cítrico	192073009	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886003	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH...	Ácido cítrico	22002309004	1
Caesar & Loretz GmbH...	Ácido cítrico	18306909	2
Caesar & Loretz GmbH...	Ácido cítrico	18306911	1
Caesar & Loretz GmbH...	Ácido cítrico	20003515003	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886002	2
Caesar & Loretz GmbH...	Ácido cítrico	21000543005	2
Caesar & Loretz GmbH...	Ácido cítrico	21000543006	4
Caesar & Loretz GmbH...	Ácido cítrico	18306906	2
Caesar & Loretz GmbH...	Ácido cítrico	18306908	1
Caesar & Loretz GmbH...	Ácido cítrico	192073003	4
Caesar & Loretz GmbH...	Ácido cítrico	21000543002	3
Caesar & Loretz GmbH...	Ácido cítrico	21000543008	2
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Ácido cítrico	21002657002	1
Caesar & Loretz GmbH/P	Ácido cítrico	192073002	1
Caesar & Loretz GmbH...	Ácido cítrico	18097611	3
Caesar & Loretz GmbH...	Ácido cítrico	18306905	1
Caesar & Loretz GmbH...	Ácido cítrico	2000886003	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH...	Ácido cítrico	21002657002	1
Caesar & Loretz GmbH...	Ácido cítrico	21000543006	1
Caesar & Loretz GmbH...	Ácido cítrico	18097606	1
Caesar & Loretz GmbH...	Ácido cítrico	18306906	1
Caesar & Loretz GmbH...	Ácido cítrico	18306908	1
Caesar & Loretz GmbH...	Ácido cítrico	18307104	1
Caesar & Loretz GmbH...	Ácido cítrico	192073002	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886007	1
Caesar & Loretz GmbH...	Ácido cítrico	20000886009	1
Caesar & Loretz GmbH...	Ácido cítrico	21000543008	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH...	Ácido cítrico	21002657002	1
Caesar & Loretz GmbH...	Ácido cítrico	21002657015	1
Caesar & Loretz GmbH...	Ácido cítrico	192073002	1
Caesar & Loretz GmbH/Sa	Ácido cítrico	192073003	2
Caesar & Loretz GmbH...	Ácido cítrico	192036004	1
Caesar & Loretz GmbH/Sana	Ácido cítrico	20000886009	1
Caesar & Loretz GmbH...	Ácido cítrico	192036009	1
Caesar & Loretz GmbH...	Ácido cítrico	18306909	1
Caesar & Loretz GmbH...	Ácido cítrico	18312104	2
Caesar & Loretz GmbH...	Ácido cítrico	192073003	1
Caesar & Loretz GmbH...	Ácido cítrico	20003515003	1
Caesar & Loretz GmbH...	Ácido cítrico	21000544002	1
Caesar & Loretz GmbH...	Ácido cítrico	21002657001	1
Caesar & Loretz GmbH/Sani	Ácido cítrico	20003515003	1
Caesar & Loretz GmbH	Ácido cítrico	13243201	1
Caesar & Loretz GmbH	Ácido cítrico	13243214	1
Caesar & Loretz GmbH	Ácido cítrico	15063003	2
Caesar & Loretz GmbH	Ácido cítrico	15063203	1
Caesar & Loretz GmbH	Ácido cítrico	16208607	1
Caesar & Loretz GmbH	Ácido cítrico	16208614	1
Caesar & Loretz GmbH	Ácido cítrico	162154403	1
Caesar & Loretz GmbH	Ácido cítrico	17162602	1
Caesar & Loretz GmbH	Ácido cítrico	17162701	1
Caesar & Loretz GmbH	Ácido cítrico	17329502	1
Caesar & Loretz GmbH	Ácido cítrico	18025701	1
Caesar & Loretz GmbH	Ácido cítrico	18097606	1
Caesar & Loretz GmbH	Ácido cítrico	18097611	2
Caesar & Loretz GmbH	Ácido cítrico	18129204	1
Caesar & Loretz GmbH	Ácido cítrico	18129205	2
Caesar & Loretz GmbH	Ácido cítrico	18129207	1
Caesar & Loretz GmbH	Ácido cítrico	18306902	5
Caesar & Loretz GmbH	Ácido cítrico	18306903	7
Caesar & Loretz GmbH	Ácido cítrico	18306904	2
Caesar & Loretz GmbH	Ácido cítrico	18306905	17
Caesar & Loretz GmbH	Ácido cítrico	18306906	13
Caesar & Loretz GmbH	Ácido cítrico	18306908	3
Caesar & Loretz GmbH	Ácido cítrico	18306909	13
Caesar & Loretz GmbH	Ácido cítrico	18306911	15
Caesar & Loretz GmbH	Ácido cítrico	18307102	2
Caesar & Loretz GmbH	Ácido cítrico	18307104	4
Caesar & Loretz GmbH	Ácido cítrico	18312103	1
Caesar & Loretz GmbH	Ácido cítrico	18312104	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ácido cítrico	18312107	2
Caesar & Loretz GmbH	Ácido cítrico	18312109	1
Caesar & Loretz GmbH	Ácido cítrico	18F25-B02	1
Caesar & Loretz GmbH	Ácido cítrico	18F25-B02_351454	1
Caesar & Loretz GmbH	Ácido cítrico	192036002	2
Caesar & Loretz GmbH	Ácido cítrico	192036003	18
Caesar & Loretz GmbH	Ácido cítrico	192036004	2
Caesar & Loretz GmbH	Ácido cítrico	192036009	1
Caesar & Loretz GmbH	Ácido cítrico	192073002	10
Caesar & Loretz GmbH	Ácido cítrico	192073003	4
Caesar & Loretz GmbH	Ácido cítrico	192073004	8
Caesar & Loretz GmbH	Ácido cítrico	192073005	10
Caesar & Loretz GmbH	Ácido cítrico	192073009	8
Caesar & Loretz GmbH	Ácido cítrico	192073010	4
Caesar & Loretz GmbH	Ácido cítrico	19H23-B07	1
Caesar & Loretz GmbH	Ácido cítrico	200000886003	1
Caesar & Loretz GmbH	Ácido cítrico	20000886002	16
Caesar & Loretz GmbH	Ácido cítrico	20000886003	7
Caesar & Loretz GmbH	Ácido cítrico	20000886007	7
Caesar & Loretz GmbH	Ácido cítrico	20000886008	3
Caesar & Loretz GmbH	Ácido cítrico	20000886009	13
Caesar & Loretz GmbH	Ácido cítrico	20003515002	2
Caesar & Loretz GmbH	Ácido cítrico	20003515003	4
Caesar & Loretz GmbH	Ácido cítrico	20003515004	1
Caesar & Loretz GmbH	Ácido cítrico	20003515008	1
Caesar & Loretz GmbH	Ácido cítrico	20003515010	2
Caesar & Loretz GmbH	Ácido cítrico	20003515014	2
Caesar & Loretz GmbH	Ácido cítrico	21000020004	1
Caesar & Loretz GmbH	Ácido cítrico	210000544002	1
Caesar & Loretz GmbH	Ácido cítrico	21000543002	2
Caesar & Loretz GmbH	Ácido cítrico	21000543003	6
Caesar & Loretz GmbH	Ácido cítrico	21000543005	4
Caesar & Loretz GmbH	Ácido cítrico	21000543008	5
Caesar & Loretz GmbH	Ácido cítrico	21000543010	6
Caesar & Loretz GmbH	Ácido cítrico	21000543011	1
Caesar & Loretz GmbH	Ácido cítrico	21000544001	6
Caesar & Loretz GmbH	Ácido cítrico	21000544002	20
Caesar & Loretz GmbH	Ácido cítrico	21000544004	13
Caesar & Loretz GmbH	Ácido cítrico	21000544006	4
Caesar & Loretz GmbH	Ácido cítrico	21002657001	4
Caesar & Loretz GmbH	Ácido cítrico	21002657002	3
Caesar & Loretz GmbH	Ácido cítrico	21002657003	11
Caesar & Loretz GmbH	Ácido cítrico	21002657006	3
Caesar & Loretz GmbH	Ácido cítrico	21002657015	3
Caesar & Loretz GmbH	Ácido cítrico	21002657016	1
Caesar & Loretz GmbH	Ácido cítrico	2100543003	1
Caesar & Loretz GmbH	Ácido cítrico	22000645001	3
Caesar & Loretz Hilden	Ácido cítrico	18312104	1
Caesar & Loretz Hilden	Ácido cítrico	18312109	1
Caesar & Loretz/ Noweda	Ácido cítrico	12156812	1
Caesar & Loretz/Geil...	Ácido cítrico	20003515003	1
Caesar & Loretz/Noweda	Ácido cítrico	20003515003	1
Caesar & Loretz	Ácido cítrico	15087904	2
Caesar & Loretz	Ácido cítrico	16038613	1
Caesar & Loretz	Ácido cítrico	18097603	1
Caesar & Loretz	Ácido cítrico	18307102	1
Caesar / Gehe	Ácido cítrico	15087904	1
Caesar u. Loretz GmbH	Ácido cítrico	18307104	1
Caesar u. Loretz GmbH	Ácido cítrico	192073005	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar u. Loretz GmbH	Ácido cítrico	21000544001	1
Caesar und Loretz	Ácido cítrico	18306911	1
Caesar&Lorenz	Ácido cítrico	21000544002	1
Caesar&Loretz GmbH,1...	Ácido cítrico	16004706	1
Caesar&Loretz GmbH	Ácido cítrico	15063213	1
Caesar&Loretz GmbH	Ácido cítrico	16038604	1
Caesar&Loretz GmbH	Ácido cítrico	22000645001	1
Caesar&loretz,Phoenix	Ácido cítrico	13243201	1
Caesar&Loretz/Geilen...	Ácido cítrico	18312104	1
Caesar/Lorenz	Ácido cítrico	13050610	1
Caleo/ Noweda	Ácido cítrico	18097607	1
Caleo/Fiebig	Ácido cítrico	18025704	1
Caleo	Ácido cítrico	16038613	1
Caolo- Noweda	Ácido cítrico	15063213	1
Cealo / Otto Geilenk...	Ácido cítrico	18306909	1
Cealo/AHD	Ácido cítrico	16038704	1
Cealo/Anzag	Ácido cítrico	16208607	1
Cealo/Gehe	Ácido cítrico	14186301	6
Cealo/Sanacorp	Ácido cítrico	17329502	1
Cealo	Ácido cítrico	16004701	1
Cordes/Noweda	Ácido cítrico	16208607	1
E Plus	Ácido cítrico	16208613	1
Ebert & Jacobi 12...	Ácido cítrico	1506214	1
Ebert & Jacobi	Ácido cítrico	16215403	1
Ebert & Jacobi	Ácido cítrico	6493071	1
Ebert-Jacobi	Ácido cítrico	16208607	1
Eu Rho	Ácido cítrico	L1202001-01	1
EuRho/Alliance Healthcare	Ácido cítrico	L1609021-02	1
EuRho/Phönix	Ácido cítrico	L1408011-02	1
EuRho	Ácido cítrico	L1503027-02	2
euro / Phoenix 19.02.2018	Ácido cítrico	11609021	1
Euro OTC	Ácido cítrico		6
Euro OTC	Ácido cítrico	1011047-03	2
Euro OTC	Ácido cítrico	1018M-01024	1
Euro OTC	Ácido cítrico	1018M-0124	1
Euro OTC	Ácido cítrico	1275983	2
Euro OTC	Ácido cítrico	13175410	1
Euro OTC	Ácido cítrico	13396515	1
Euro OTC	Ácido cítrico	13K18-B34	1
Euro OTC	Ácido cítrico	1406014-02	1
Euro OTC	Ácido cítrico	150317-965	1
Euro OTC	Ácido cítrico	1505029B	1
Euro OTC	Ácido cítrico	16004702	1
Euro OTC	Ácido cítrico	16038713	1
Euro OTC	Ácido cítrico	17162601	2
Euro OTC	Ácido cítrico	17329502	1
Euro OTC	Ácido cítrico	2112002-01	1
Euro OTC	Ácido cítrico	2301021-01	1
Euro OTC	Ácido cítrico	702260	5
Euro OTC	Ácido cítrico	Intern-Ch1018M-01024	1
Euro OTC	Ácido cítrico	L1202001-01	5
Euro OTC	Ácido cítrico	L1202001-02	1
Euro OTC	Ácido cítrico	L130404201	2
Euro OTC	Ácido cítrico	L1304042-01	2
Euro OTC	Ácido cítrico	L1304042-02	1
Euro OTC	Ácido cítrico	L1408011-01	2
Euro OTC	Ácido cítrico	L1408011-02	2
Euro OTC	Ácido cítrico	L1503027-01	1
Euro OTC	Ácido cítrico	L1503027-02	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Ácido cítrico	L1508013-01	4
Euro OTC	Ácido cítrico	L1508013-02	1
Euro OTC	Ácido cítrico	L1604061-02	5
Euro OTC	Ácido cítrico	l1604062-01	1
Euro OTC	Ácido cítrico	L160461-02	1
Euro OTC	Ácido cítrico	L1609021-01	6
Euro OTC	Ácido cítrico	L1609021-02	4
Euro OTC	Ácido cítrico	L1805017-01	2
Euro OTC	Ácido cítrico	L1812017-01	5
Euro OTC	Ácido cítrico	L1812017-02	1
Euro OTC	Ácido cítrico	L2002036-01	2
Euro OTC	Ácido cítrico	L2002036-02	1
Euro OTC	Ácido cítrico	L2010013-01	1
Fagron	Ácido cítrico		1
Fagron	Ácido cítrico	100614d	1
Fagron	Ácido cítrico	10G21-N05	2
Fagron	Ácido cítrico	1151608	2
Fagron	Ácido cítrico	1155609	9
Fagron	Ácido cítrico	1156158	1
Fagron	Ácido cítrico	1172673	10
Fagron	Ácido cítrico	1181765	3
Fagron	Ácido cítrico	11C24-N02	3
Fagron	Ácido cítrico	11C24N022869/4250	1
Fagron	Ácido cítrico	11C24-N03	6
Fagron	Ácido cítrico	11H30-N05	1
Fagron	Ácido cítrico	11K07N01	1
Fagron	Ácido cítrico	11K07-N01	7
Fagron	Ácido cítrico	11K11-N02	2
Fagron	Ácido cítrico	11K11-N020444/1975	1
Fagron	Ácido cítrico	12175711	1
Fagron	Ácido cítrico	12801-N01	1
Fagron	Ácido cítrico	12b01-N01	1
Fagron	Ácido cítrico	12B01N01	1
Fagron	Ácido cítrico	12B01-N01	23
Fagron	Ácido cítrico	12B01-No1	1
Fagron	Ácido cítrico	12B01-NO1	1
Fagron	Ácido cítrico	12BO1-N01	1
Fagron	Ácido cítrico	12F06-M06	3
Fagron	Ácido cítrico	13804-N02	1
Fagron	Ácido cítrico	13A04N04	1
Fagron	Ácido cítrico	13A04-N04	13
Fagron	Ácido cítrico	13A-04-N04	2
Fagron	Ácido cítrico	13A04-N040019/4900	1
Fagron	Ácido cítrico	13A04-NO4	1
Fagron	Ácido cítrico	13B04-N01	1
Fagron	Ácido cítrico	13F12-N01	3
Fagron	Ácido cítrico	13F12-N08	1
Fagron	Ácido cítrico	13G04-N05	5
Fagron	Ácido cítrico	13G24N13	2
Fagron	Ácido cítrico	13G24-N13	6
Fagron	Ácido cítrico	13G24-N24	13
Fagron	Ácido cítrico	13G24-N240029/900	1
Fagron	Ácido cítrico	13G24-N240739/900	1
Fagron	Ácido cítrico	13H22-N09	2
Fagron	Ácido cítrico	13K18-B34	5
Fagron	Ácido cítrico	13K18-B34_291522	1
Fagron	Ácido cítrico	13K18-B34-288371	4
Fagron	Ácido cítrico	13k18-B34-288372	1
Fagron	Ácido cítrico	13K18-B34-288372	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ácido cítrico	13K18-B34-288373	1
Fagron	Ácido cítrico	13K18-B34-291071	4
Fagron	Ácido cítrico	13K18-B34-291072	2
Fagron	Ácido cítrico	13K18-B34-291519	5
Fagron	Ácido cítrico	13K18-B34-291520	4
Fagron	Ácido cítrico	13K18-B34-291521	4
Fagron	Ácido cítrico	13k18-b34-291522	1
Fagron	Ácido cítrico	13K18-B34-291522	6
Fagron	Ácido cítrico	13K18-B34-291523	2
Fagron	Ácido cítrico	13K18-B34-293871	2
Fagron	Ácido cítrico	13L05-B02-296246	3
Fagron	Ácido cítrico	13L05B02296247	1
Fagron	Ácido cítrico	13L05-B02-309050	1
Fagron	Ácido cítrico	13L18-B39-289347	4
Fagron	Ácido cítrico	14b06-b07-293872	1
Fagron	Ácido cítrico	14E06-B07293872	1
Fagron	Ácido cítrico	14E06-B07-293872	4
Fagron	Ácido cítrico	14E06-B07293873	1
Fagron	Ácido cítrico	14E06-B07-293873	1
Fagron	Ácido cítrico	14E06-B07-293875	3
Fagron	Ácido cítrico	14E06-B07-293890	4
Fagron	Ácido cítrico	14E-06-B07-293890	1
Fagron	Ácido cítrico	14G04-B09-293874	11
Fagron	Ácido cítrico	14G04-b09-293876	1
Fagron	Ácido cítrico	14G04B09293876	1
Fagron	Ácido cítrico	14G04-B09-293876	4
Fagron	Ácido cítrico	14g04-b09293877	1
Fagron	Ácido cítrico	14G04-B09-293877	12
Fagron	Ácido cítrico	14G04-B09-296361	1
Fagron	Ácido cítrico	14G04-B09-309707	1
Fagron	Ácido cítrico	14G04-B09-309836	3
Fagron	Ácido cítrico	14K05_B04_302815	1
Fagron	Ácido cítrico	14K05-B04-302815	6
Fagron	Ácido cítrico	14k05-b04-302816	1
Fagron	Ácido cítrico	14K05-B04-302816	6
Fagron	Ácido cítrico	14K05-B04-302817	2
Fagron	Ácido cítrico	14K05-B04-302826	1
Fagron	Ácido cítrico	15044902	1
Fagron	Ácido cítrico	15G16b01	1
Fagron	Ácido cítrico	15G16B01	1
Fagron	Ácido cítrico	15G16-B01	2
Fagron	Ácido cítrico	15G16-B01330449	2
Fagron	Ácido cítrico	15G16-B01-330449	16
Fagron	Ácido cítrico	15g16-b01-330450	2
Fagron	Ácido cítrico	15G16B01330450	1
Fagron	Ácido cítrico	15G16-B01330450	1
Fagron	Ácido cítrico	15G16-B01-330450	8
Fagron	Ácido cítrico	15G16-B01-330450	1
Fagron	Ácido cítrico	15l01-B06-324348	1
Fagron	Ácido cítrico	16072014B	1
Fagron	Ácido cítrico	16208607	1
Fagron	Ácido cítrico	1714Q1024	1
Fagron	Ácido cítrico	17E15-B04	2
Fagron	Ácido cítrico	17E15-B04-335435	3
Fagron	Ácido cítrico	17E15-B04-341741	1
Fagron	Ácido cítrico	17E15-B04-345678	6
Fagron	Ácido cítrico	17E15-B04-345679	3
Fagron	Ácido cítrico	17E15-B04-347168	3
Fagron	Ácido cítrico	17E15-B04-347169	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ácido cítrico	18F25-B02	1
Fagron	Ácido cítrico	18F25-B02-351448	1
Fagron	Ácido cítrico	18F25-B02-351454	1
Fagron	Ácido cítrico	18F25-B02-355281	3
Fagron	Ácido cítrico	18F25-B02-355298	2
Fagron	Ácido cítrico	1913A-01024	1
Fagron	Ácido cítrico	19B06-B02-191458	1
Fagron	Ácido cítrico	19h23-B07-194438	1
Fagron	Ácido cítrico	19H23-B07-194438	4
Fagron	Ácido cítrico	19H23B07194441	1
Fagron	Ácido cítrico	19H23-B07-200458	1
Fagron	Ácido cítrico	19H23-Bo7-200458	1
Fagron	Ácido cítrico	20071203	1
Fagron	Ácido cítrico	20F16-B02-201199	1
Fagron	Ácido cítrico	20G31-B01-201878	3
Fagron	Ácido cítrico	20L01-B10-202958	2
Fagron	Ácido cítrico	214U-01024	1
Fagron	Ácido cítrico	21F00-B04-218885	1
Fagron	Ácido cítrico	21F11-804-218885	1
Fagron	Ácido cítrico	21F11-B03-216679	1
Fagron	Ácido cítrico	21F11-B04-213768	2
Fagron	Ácido cítrico	21F11-B04-218885	2
Fagron	Ácido cítrico	21F11-B04-221484	1
Fagron	Ácido cítrico	22031401	1
Fagron	Ácido cítrico	22G15-B05-220815	1
Fagron	Ácido cítrico	26082013B	1
Fagron	Ácido cítrico	28021404	1
Fagron	Ácido cítrico	20F16-B02_201199	1
Fagron	Ácido cítrico	330449	1
Fagron	Ácido cítrico	351453	1
Fagron	Ácido cítrico	4810E-01024	1
Fagron	Ácido cítrico	6496091	1
Fagron	Ácido cítrico	700309-0001	1
Fagron	Ácido cítrico	700309-0003	2
Fagron	Ácido cítrico	700309-0006	1
Fagron	Ácido cítrico	700309-001	1
Fagron	Ácido cítrico	7200458	1
Fagron	Ácido cítrico	L1604061-02	1
Fagron	Ácido cítrico	L1812017-01	2
Fagron	Ácido cítrico	probe	1
Fagron	Ácido cítrico	UJ051	1
Fagron	Ácido cítrico	UJ501	2
Fargon/Sanacorp	Ácido cítrico		1
Fargon	Ácido cítrico	12B01-N01	1
Fargon	Ácido cítrico	12B01-NN01	1
fargon	Ácido cítrico	13A04-N04	1
Faron	Ácido cítrico	UJ45	1
Fiebig	Ácido cítrico	13243201	1
Fiebig	Ácido cítrico	14K05-B04-302815	1
Fiebig	Ácido cítrico	15063204	1
Fiebig	Ácido cítrico	17162702	1
Finze	Ácido cítrico	12156812	2
Fischar/Noweda	Ácido cítrico	6494061	1
Fischar/Phönix	Ácido cítrico	6497051	2
Fischar	Ácido cítrico	649061	2
fischar	Ácido cítrico	6491041	1
Fischar	Ácido cítrico	6493071	1
Fischar	Ácido cítrico	6494061	2
Fischar	Ácido cítrico	6496091	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fischar	Ácido cítrico	6498011	2
Fischar	Ácido cítrico	6499061	1
Fischer/Noweda	Ácido cítrico	6496091	1
fishar	Ácido cítrico	6494061	1
Fragon/Phoenix	Ácido cítrico	14G04-B09-293976	1
Fragon/Phönix	Ácido cítrico	18F25-B02-351463	1
Fragron/Noweda	Ácido cítrico	15G16-B01-330449	1
GEHE 02.07.2014	Ácido cítrico	13243217	1
Gehe 21-01-2019	Ácido cítrico	18097609	1
Gehe amax	Ácido cítrico	18129205	1
Gehe amax	Ácido cítrico	192036003	1
Gehe Kassel, 22.05.2015	Ácido cítrico	14E06-B07-293872	1
Gehe Rostock	Ácido cítrico	21000543006	1
Gehe/Euro	Ácido cítrico	160406-02	1
Gehe/Fragon	Ácido cítrico	14G04B09293876	1
Gehe	Ácido cítrico	11C24-N02	1
Gehe	Ácido cítrico	11C24-N03	2
Gehe	Ácido cítrico	11K07-N01	2
Gehe	Ácido cítrico	12043111	1
Gehe	Ácido cítrico	13175403	1
Gehe	Ácido cítrico	13175404	1
Gehe	Ácido cítrico	15044902	1
Gehe	Ácido cítrico	15063003	1
Gehe	Ácido cítrico	15063203	1
Gehe	Ácido cítrico	15063217	1
Gehe	Ácido cítrico	15087902	1
Gehe	Ácido cítrico	15G16-B01-330450	1
Gehe	Ácido cítrico	16004706	1
Gehe	Ácido cítrico	16038614	1
GEHE	Ácido cítrico	16208606	1
Gehe	Ácido cítrico	16208612	1
Gehe	Ácido cítrico	17162601	2
Gehe	Ácido cítrico	17162602	1
Gehe	Ácido cítrico	17162603	1
Gehe	Ácido cítrico	18097607	1
GEHE	Ácido cítrico	18097607	1
GEHE	Ácido cítrico	18097611	1
Gehe	Ácido cítrico	18306906	1
Gehe	Ácido cítrico	18307102	1
Gehe	Ácido cítrico	192073009	1
Gehe	Ácido cítrico	20000886003	1
Gehe	Ácido cítrico	21000544001	1
Gehe	Ácido cítrico	21002657003	1
GEHE	Ácido cítrico	21002657003	1
Gehe	Ácido cítrico	22000645011	1
GEHE	Ácido cítrico	22000645011	1
Gehe	Ácido cítrico	22002309001	1
Geilenkirchen	Ácido cítrico	16208606	1
Geilenkirchen	Ácido cítrico	18306906	1
Geilenkirchen	Ácido cítrico	21000544002	1
Hedinger	Ácido cítrico	18306906	1
Henry Lamotte Oils GmbH	Ácido cítrico		1
Hepart	Ácido cítrico	16208614	1
Ichthyol	Ácido cítrico	16038608	1
Ichtyhol Gesellschaf...	Ácido cítrico	16038618	1
Jenne 05.11.21 EK:6,97EUR	Ácido cítrico	211108C	1
Jenne	Ácido cítrico	15063002	1
Jenne	Ácido cítrico	200000886007	1
Jungbunzlauer Ladenb...	Ácido cítrico	1156158	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Jungbunzlauer Ladenb…	Ácido cítrico	1155609	1
Kehr.21.07.2020	Ácido cítrico	192073004	1
Kehr.28.04.2020	Ácido cítrico	192073005	2
Kehr	Ácido cítrico	17162602	1
Kehr	Ácido cítrico	22002250001	1
Kehr	Ácido cítrico	22002309004	1
Klenk	Ácido cítrico	12B01-N01	2
Klenk	Ácido cítrico	13243201	1
Krieger	Ácido cítrico	21002657015	1
L10	Ácido cítrico	9494185	1
Lamotte	Ácido cítrico	15063213	1
Merck	Ácido cítrico		1
Merck	Ácido cítrico	K53604941	1
Nachtestung-Verlängerung	Ácido cítrico	278/18	1
Noweda 13.6.2019	Ácido cítrico	18306905	2
Noweda	Ácido cítrico	12043110	1
Noweda	Ácido cítrico	13050601	1
Noweda	Ácido cítrico	13050621	1
Noweda	Ácido cítrico	13243216	1
Noweda	Ácido cítrico	15063203	1
Noweda	Ácido cítrico	15087902	2
Noweda	Ácido cítrico	16004701	1
Noweda	Ácido cítrico	16208606	3
Noweda	Ácido cítrico	16208607	1
Noweda	Ácido cítrico	16208614	1
Noweda	Ácido cítrico	18025701	1
Noweda	Ácido cítrico	18025704	1
Noweda	Ácido cítrico	18097606	1
Noweda	Ácido cítrico	18306903	1
Noweda	Ácido cítrico	18306906	2
Noweda	Ácido cítrico	18306911	1
Noweda	Ácido cítrico	18307102	1
Noweda	Ácido cítrico	18312104	1
Noweda	Ácido cítrico	20000886002	1
Noweda	Ácido cítrico	20000886009	1
Noweda	Ácido cítrico	21000543008	1
Noweda	Ácido cítrico	21000543010	1
Noweda	Ácido cítrico	21002657003	1
Noweda	Ácido cítrico	21002657015	2
Noweda	Ácido cítrico	21002657016	1
Noweda	Ácido cítrico	21002657017	1
Noweda	Ácido cítrico	22000645001	1
Noweda	Ácido cítrico	22000645005	1
Noweda	Ácido cítrico	22002309004	1
Noweda	Ácido cítrico	L1202001-02	1
O.Fischer GmbH/Anzag…	Ácido cítrico	6498011	1
Otto Fischar GmbH&Co KG	Ácido cítrico	6496091	1
Otto Fischar GmbH&Co. KG	Ácido cítrico	6494061	6
Otto Fischar GmbH&Co. KG	Ácido cítrico	6496051	1
Otto Fischar GmbH/ N…	Ácido cítrico	6494061	1
Otto Fischar GmbH	Ácido cítrico	6498011	1
Otto Fischar/Kehr	Ácido cítrico	6498011	1
Otto Fischar	Ácido cítrico	6494061	1
Otto Fischar	Ácido cítrico	6498011	1
Otto Fischer / Sana	Ácido cítrico	6493071	1
Otto Fischer GmbH & …	Ácido cítrico	6496091	1
Otto Fischer GmbH/Sana	Ácido cítrico	6497051	1
Otto Fischer GmbH	Ácido cítrico	6492061	1
Otto Fishar	Ácido cítrico	6496091	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix 07.04.2014	Ácido cítrico	13A04-N04	1
Phoenix 12.12.2016 4,59EUR	Ácido cítrico	1508808	1
Phoenix 14.08.2017	Ácido cítrico	16038712	1
Phoenix 29.05.2019 2,48EUR	Ácido cítrico	18306902	1
Phoenix 31.01.2019	Ácido cítrico	18097607	1
phoenix 5.6.14	Ácido cítrico	1172673	1
Phoenix	Ácido cítrico	1172673	1
Phoenix	Ácido cítrico	12b01-N01	1
Phoenix	Ácido cítrico	13243202	1
Phoenix	Ácido cítrico	13K18-B34-288372	1
Phoenix	Ácido cítrico	16208606	1
Phoenix	Ácido cítrico	16208614	1
Phoenix	Ácido cítrico	18025701	1
Phoenix	Ácido cítrico	18097603	1
Phoenix	Ácido cítrico	18097607	1
Phoenix	Ácido cítrico	18306911	1
Phoenix	Ácido cítrico	19B06-B02-191458	1
Phoenix	Ácido cítrico	20000886009	1
Phoenix	Ácido cítrico	21000544002	2
Phoenix	Ácido cítrico	21002657015	1
Phoenix	Ácido cítrico	22000645011	1
Phoenix	Ácido cítrico	22002309004	1
Phoenix	Ácido cítrico	2310005-01	1
Phönix Gotha	Ácido cítrico	12B01-N011973/6000	1
Phönix Gotha	Ácido cítrico	12B01-N012028/6000	1
Phönix Gotha	Ácido cítrico	12B01-N012125/6000	1
Phönix Gotha	Ácido cítrico	13050609	1
Phönix Gotha	Ácido cítrico	13050618	1
Phönix Gotha	Ácido cítrico	13A04-N040049-100	1
Phönix Gotha	Ácido cítrico	15063206	2
Phönix/Fagon	Ácido cítrico	14604-B09-293876	1
Phönix/Gehe	Ácido cítrico	16208614	1
Phönix	Ácido cítrico	10005440022	1
Phönix	Ácido cítrico	1155609	1
Phönix	Ácido cítrico	123456	1
Phönix	Ácido cítrico	13A04-N04	1
Phönix	Ácido cítrico	14186312	4
Phönix	Ácido cítrico	15063213	1
phönix	Ácido cítrico	16038604	3
phönix	Ácido cítrico	16208608	1
Phönix	Ácido cítrico	16208613	1
Phönix	Ácido cítrico	16215406	1
Phönix	Ácido cítrico	18025702	2
Phönix	Ácido cítrico	18025704	1
Phönix	Ácido cítrico	18097601	1
Phönix	Ácido cítrico	18097603	3
Phönix	Ácido cítrico	18097607	1
Phönix	Ácido cítrico	192073003	1
Phönix	Ácido cítrico	192073005	1
Phönix	Ácido cítrico	20000886002	1
Phönix	Ácido cítrico	20000886003	1
Phönix	Ácido cítrico	20000886009	1
Phönix	Ácido cítrico	21000543002	1
Phönix	Ácido cítrico	21000543011	1
Phönix	Ácido cítrico	21000544004	1
Phönix	Ácido cítrico	21002657003	1
Sanacorb;20.04.15; 7,45EUR	Ácido cítrico	1375410	1
Sanacorp/Bionorica Ethics	Ácido cítrico	16038622	1
Sanacorp	Ácido cítrico	12156811	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Ácido cítrico	12156823	1
Sanacorp	Ácido cítrico	12156824	1
Sanacorp	Ácido cítrico	12156832	1
Sanacorp	Ácido cítrico	1216832	1
Sanacorp	Ácido cítrico	13050604	1
Sanacorp	Ácido cítrico	13243214	1
sanacorp	Ácido cítrico	13396505	1
Sanacorp	Ácido cítrico	13K18-B34-291072	1
Sanacorp	Ácido cítrico	15i01-b06-324348	1
Sanacorp	Ácido cítrico	16208608	1
Sanacorp	Ácido cítrico	16208614	1
Sanacorp	Ácido cítrico	17162601	5
Sanacorp	Ácido cítrico	18025702	1
Sanacorp	Ácido cítrico	18025704	1
Sanacorp	Ácido cítrico	18097603	1
Sanacorp	Ácido cítrico	183066905	1
Sanacorp	Ácido cítrico	18306909	1
Sanacorp	Ácido cítrico	192073004	1
Sanacorp	Ácido cítrico	192073005	1
Sanacorp	Ácido cítrico	20000886002	1
Sanacorp	Ácido cítrico	20003515003	1
Sanacorp	Ácido cítrico	21000543011	3
Sanacorp	Ácido cítrico	21000544001	1
Sanacorp	Ácido cítrico	21002657015	2
Sanacorp	Ácido cítrico	22000645004	1
Sanacorp	Ácido cítrico	22002309001	2
Sanacorp	Ácido cítrico	22002309004	1
Sanacorp	Ácido cítrico	40/AKD2	1
Sanacorp	Ácido cítrico	41/AKD4	1
SanacorpWE:15.02.201…	Ácido cítrico	15063203	1
SanacorpWE:30.01.201…	Ácido cítrico	16038707	1
Spangropharm	Ácido cítrico	13050611	3
VDL 16.03.15; 2,54EUR	Ácido cítrico	13243201	1
VDL;23.6.14; 2.49EUR	Ácido cítrico	13243213	1
Wolf Apotheke	Ácido cítrico	58(18097609)	1

- 231 724 spectra from 1513 *Apo-Ident* customers from a total of 48 608 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido cítrico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido cítrico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	1170	0	200 914
Type C	0	4319	24	231 724

The substance/substance group *Ácido cítrico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4872 %)
Type C	100.0000 % (> 99.9007 %)	99.4474 % (> 99.3783 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20682	22463	20,26	98,56
20683	22463	5,50	111,16
20706	22463	19,43	99,00
20913	22463	5,43	123,72
21455	22463	23,26	97,83
21487	22463	14,74	103,95
22463	22463	0,00	118,38
26350	26350	0,00	114,01

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido cítrico monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20012-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido cítrico monoidratado; Acidum citricum monohydricum

Special notes

When selecting the *Ácido cítrico monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido cítrico monoidratado	8	4	109

Second-stage model

For differentiation of the substance/substance group *Ácido cítrico monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido cítrico monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	86,83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido cítrico monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido cítrico monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido cítrico monoidratado	15185301	22340	60	20150708
Caelo	Ácido cítrico monoidratado	17085602	23409	40	20170410
Caelo	Ácido cítrico monoidratado	181305	24222	40	20180606*
Caelo	Ácido cítrico monoidratado	19000762	25563	40	20200204*
Caelo	Ácido cítrico monoidratado	23001973	26954	40	20231108*
Caelo	Ácido cítrico monoidratado	23001973	26954SI	20	20231108*
Fagron	Ácido cítrico monoidratado	12D26-N02	20926	40	20120515
Hedinger	Ácido cítrico monoidratado	202029	23457	40	20161110
Hedinger	Ácido cítrico monoidratado	202029	23458	40	1908675
Hedinger	Ácido cítrico monoidratado	202030	24874	40	20180727

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Ácido cítrico monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Ácido cítrico monoidratado*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido cítrico monoidratado	161865	22617	40
Caelo	Ácido cítrico monoidratado	21001368	25796	50
Caelo	Ácido cítrico monoidratado	22001438	26121	40
Caelo	Ácido cítrico monoidratado	23001974	26948	40
Caelo	Ácido cítrico monoidratado	161865	23298	40
Caelo	Ácido cítrico monoidratado	22001438	26121SI	20
Caelo	Ácido cítrico monoidratado	23001974	26948SI	20

- 201 834 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 409 spectra from 186 *Apo-Ident* customers from 113 batches from the substance/substance group *Ácido cítrico monoidratado*.

- Among them are spectra of independent samples from 105 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido cítrico monoidratado	22001438007	4
AEP	Ácido cítrico monoidratado	190884005	1
AHD	Ácido cítrico monoidratado	22001438007	2
AHD	Ácido cítrico monoidratado	23003303002	1
Alliance Healthcare	Ácido cítrico monoidratado	18130503	1
Bombastus	Ácido cítrico monoidratado		1
Bombastus	Ácido cítrico monoidratado	18000110	1
Bombastus	Ácido cítrico monoidratado	18003283	1
Bombastus	Ácido cítrico monoidratado	18003407	1
Bombastus	Ácido cítrico monoidratado	201-069-1	2
Bombastus	Ácido cítrico monoidratado	259437	1
Bombastus	Ácido cítrico monoidratado	294630	1
Bombastus	Ácido cítrico monoidratado	309343	1
Bombastus	Ácido cítrico monoidratado	309344	2
Bombastus	Ácido cítrico monoidratado	309650	1
Bombastus	Ácido cítrico monoidratado	310803	2
Bombastus	Ácido cítrico monoidratado	70620101	1
Caelo	Ácido cítrico monoidratado	11208132	3
Caelo	Ácido cítrico monoidratado	11208133	4
Caelo	Ácido cítrico monoidratado	12125904	2
Caelo	Ácido cítrico monoidratado	12125907	6
Caelo	Ácido cítrico monoidratado	12125937	3
Caelo	Ácido cítrico monoidratado	12125938	1
Caelo	Ácido cítrico monoidratado	1212937	1
Caelo	Ácido cítrico monoidratado	1215907	1
Caelo	Ácido cítrico monoidratado	1215911	1
Caelo	Ácido cítrico monoidratado	13069103	1
Caelo	Ácido cítrico monoidratado	13069104	6
Caelo	Ácido cítrico monoidratado	13069105	2
Caelo	Ácido cítrico monoidratado	13069106	3
Caelo	Ácido cítrico monoidratado	13069110	4
Caelo	Ácido cítrico monoidratado	13069111	3
Caelo	Ácido cítrico monoidratado	13069113	2
Caelo	Ácido cítrico monoidratado	13069124	4
Caelo	Ácido cítrico monoidratado	13069125	2
Caelo	Ácido cítrico monoidratado	13069128	3
Caelo	Ácido cítrico monoidratado	13069129	4
Caelo	Ácido cítrico monoidratado	13069130	1
Caelo	Ácido cítrico monoidratado	13069133	5
Caelo	Ácido cítrico monoidratado	14038401	6
Caelo	Ácido cítrico monoidratado	14038403	8
Caelo	Ácido cítrico monoidratado	14071701	1
Caelo	Ácido cítrico monoidratado	14311807	2
Caelo	Ácido cítrico monoidratado	14311808	4
Caelo	Ácido cítrico monoidratado	14311812	4
Caelo	Ácido cítrico monoidratado	14311813	1
Caelo	Ácido cítrico monoidratado	15087502	2
Caelo	Ácido cítrico monoidratado	15087503	2
Caelo	Ácido cítrico monoidratado	15087509	9
Caelo	Ácido cítrico monoidratado	15087510	2
Caelo	Ácido cítrico monoidratado	15087512	1
Caelo	Ácido cítrico monoidratado	15185301	2
Caelo	Ácido cítrico monoidratado	15185302	14
Caelo	Ácido cítrico monoidratado	15185304	12
Caelo	Ácido cítrico monoidratado	15185309	5
Caelo	Ácido cítrico monoidratado	15185314	5
Caelo	Ácido cítrico monoidratado	15185316	6
Caelo	Ácido cítrico monoidratado	15185317	2
Caelo	Ácido cítrico monoidratado	15185320	3
Caelo	Ácido cítrico monoidratado	15185321	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido cítrico monoidratado	161865001	1
Caelo	Ácido cítrico monoidratado	16186501	5
Caelo	Ácido cítrico monoidratado	16186502	6
Caelo	Ácido cítrico monoidratado	16186508	6
Caelo	Ácido cítrico monoidratado	17085602	9
Caelo	Ácido cítrico monoidratado	17085603	8
Caelo	Ácido cítrico monoidratado	17085607	5
Caelo	Ácido cítrico monoidratado	17329801	1
Caelo	Ácido cítrico monoidratado	17329804	16
Caelo	Ácido cítrico monoidratado	17329807	1
Caelo	Ácido cítrico monoidratado	17329808	4
Caelo	Ácido cítrico monoidratado	18130503	3
Caelo	Ácido cítrico monoidratado	18130506	1
Caelo	Ácido cítrico monoidratado	18130509	1
Caelo	Ácido cítrico monoidratado	18130510	2
Caelo	Ácido cítrico monoidratado	19000762002	4
Caelo	Ácido cítrico monoidratado	1900762002	1
Caelo	Ácido cítrico monoidratado	190884001	4
Caelo	Ácido cítrico monoidratado	190884002	1
Caelo	Ácido cítrico monoidratado	190884005	10
Caelo	Ácido cítrico monoidratado	190884006	1
Caelo	Ácido cítrico monoidratado	190884008	4
Caelo	Ácido cítrico monoidratado	19088401	10
Caelo	Ácido cítrico monoidratado	19088402	3
Caelo	Ácido cítrico monoidratado	19088405	1
Caelo	Ácido cítrico monoidratado	19088407	5
Caelo	Ácido cítrico monoidratado	19088408	1
Caelo	Ácido cítrico monoidratado	20003892007	2
Caelo	Ácido cítrico monoidratado	20003892008	10
Caelo	Ácido cítrico monoidratado	20003892012	1
Caelo	Ácido cítrico monoidratado	21001368003	1
Caelo	Ácido cítrico monoidratado	21001368006	11
Caelo	Ácido cítrico monoidratado	21001368009	1
Caelo	Ácido cítrico monoidratado	21001368010	2
Caelo	Ácido cítrico monoidratado	21001368013	3
Caelo	Ácido cítrico monoidratado	22001438003	4
Caelo	Ácido cítrico monoidratado	22001438006	1
Caelo	Ácido cítrico monoidratado	22001438007	1
Caelo	Ácido cítrico monoidratado	2515Q-02959	1
Caelo	Ácido cítrico monoidratado	2x19088400	1
Caelo	Ácido cítrico monoidratado	9522496	1
Caelo	Ácido cítrico monoidratado	sjdfksjfdkl	1
Caesar & Loretz GmbH...	Ácido cítrico monoidratado	22001438003	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico monoidratado	19088401	1
Caesar & Loretz GmbH/Gehe	Ácido cítrico monoidratado	22001438003	1
Caesar & Loretz GmbH...	Ácido cítrico monoidratado	21001368006	1
Caesar & Loretz GmbH	Ácido cítrico monoidratado	18130506	1
Caesar & Loretz GmbH	Ácido cítrico monoidratado	19000762002	2
Caesar & Loretz GmbH	Ácido cítrico monoidratado	190884001	2
Caesar & Loretz GmbH	Ácido cítrico monoidratado	190884005	4
Caesar & Loretz GmbH	Ácido cítrico monoidratado	190884008	1
Caesar & Loretz GmbH	Ácido cítrico monoidratado	19088405	2
Caesar & Loretz GmbH	Ácido cítrico monoidratado	19088407	3
Caesar & Loretz GmbH	Ácido cítrico monoidratado	19088408	1
Caesar & Loretz GmbH	Ácido cítrico monoidratado	20003892002	4
Caesar & Loretz GmbH	Ácido cítrico monoidratado	20003892007	1
Caesar & Loretz GmbH	Ácido cítrico monoidratado	20003892008	4
Caesar & Loretz GmbH	Ácido cítrico monoidratado	2000392002	1
Caesar & Loretz GmbH	Ácido cítrico monoidratado	21001368006	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar &Loretz GmbH	Ácido cítrico monoidratado	12125937	1
Cealo	Ácido cítrico monoidratado	15185320	1
E Plus	Ácido cítrico monoidratado	16186508	1
Ebert 17.08.16	Ácido cítrico monoidratado	15185314	1
Euro OTC	Ácido cítrico monoidratado	17085607	1
Europharm / Gehe	Ácido cítrico monoidratado	17329804	1
Fiebig28.08.13 EK6,60	Ácido cítrico monoidratado	13069111	1
Gehe	Ácido cítrico monoidratado	17085602	1
Gehe	Ácido cítrico monoidratado	17329804	1
Gehe	Ácido cítrico monoidratado	22001438003	1
Gehe	Ácido cítrico monoidratado	22001438007	1
Geilenkirchen	Ácido cítrico monoidratado	16186502	1
Hänseler	Ácido cítrico monoidratado		4
Hedinger / Phönix	Ácido cítrico monoidratado	202029	1
Hedinger/Phönix	Ácido cítrico monoidratado	202029	1
Hedinger	Ácido cítrico monoidratado	202028	2
Hedinger	Ácido cítrico monoidratado	202029	3
Henry Lamotte/AHD	Ácido cítrico monoidratado	17329804	1
Herba Gatt Koller	Ácido cítrico monoidratado	201103153211	1
Krieger	Ácido cítrico monoidratado	613001-1-P	1
Nachprüfung	Ácido cítrico monoidratado	AP201218-07	1
Phönix	Ácido cítrico monoidratado	10111503	1
Phönix	Ácido cítrico monoidratado	1403/3	1
Sanacaorp	Ácido cítrico monoidratado	14038401	2
Sanacorp	Ácido cítrico monoidratado	1215937	1
Sanacorp	Ácido cítrico monoidratado	21001368006	1
Sanacorp	Ácido cítrico monoidratado	22001438007	1
VDL	Ácido cítrico monoidratado	263669	1

- 235 658 spectra from 1515 *Apo-Ident* customers from a total of 49 149 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido cítrico monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido cítrico monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	250	0	201 834
Type C	0	406	3	235 658

The substance/substance group *Ácido cítrico monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	99.2665 % (> 98.5330 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20926	23458	6,98	226,73
22340	26954	13,90	225,59
23409	23458	11,58	227,97
23457	26954	9,19	226,71
23458	23458	0,00	226,97
24222	24222	0,00	228,98
24874	26954	5,13	225,98
25563	25563	0,00	226,69
26954	26954	0,00	223,67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido esteárico 50**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20869-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido esteárico 50; Acidum stearicum

Special notes

When selecting the *Ácido esteárico 50* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido esteárico 50	6	4	36

Second-stage model

For differentiation of the substance/substance group *Ácido esteárico 50* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido esteárico 50* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Gordura sólida	93,84	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido esteárico 50* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido esteárico 50*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido esteárico 50	12241910	20869	40	AR-15-FG-007284-01
Caelo	Ácido esteárico 50	14359310	21793	60	20150126
Caelo	Ácido esteárico 50	14359310	21928	60	AR-16-FG-004044-01
Caelo	Ácido esteárico 50	14359314	22274	60	20150126
Caelo	Ácido esteárico 50	170810	23294	40	20170426*
Caelo	Ácido esteárico 50	170810	23667	40	20170426*
Caelo	Ácido esteárico 50	192910	25066	40	20191128*
Caelo	Ácido esteárico 50	22000750	26125	30	20220429*
Caelo	Ácido esteárico 50	22000750	26125SI	20	20220429*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 390 spectra of 9 reference samples from the substance/substance group *Ácido esteárico 50*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 572 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 5 reference samples from the substance/substance group *Ácido esteárico 50*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido esteárico 50	163469	23032	40
Caelo	Ácido esteárico 50	180809	24036	40
Caelo	Ácido esteárico 50	20003933010	25731	50
Caelo	Ácido esteárico 50	23001610	26833	40
Caelo	Ácido esteárico 50	23001610	26833SI	20

- 201 894 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 88 spectra from 42 *Apo-Ident* customers from 39 batches from the substance/substance group *Ácido esteárico 50*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido esteárico 50	23001610002	1
Caelo	Ácido esteárico 50	11103706	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido esteárico 50	11308505	1
Caelo	Ácido esteárico 50	11308514	1
Caelo	Ácido esteárico 50	12241911	2
Caelo	Ácido esteárico 50	12241914	1
Caelo	Ácido esteárico 50	12241915	2
Caelo	Ácido esteárico 50	12241930	3
Caelo	Ácido esteárico 50	14359314	4
Caelo	Ácido esteárico 50	1609611	1
Caelo	Ácido esteárico 50	16096301	2
Caelo	Ácido esteárico 50	16096311	1
Caelo	Ácido esteárico 50	1617081006	1
Caelo	Ácido esteárico 50	17081003	1
Caelo	Ácido esteárico 50	17081006	5
Caelo	Ácido esteárico 50	1808013	1
Caelo	Ácido esteárico 50	18080901	4
Caelo	Ácido esteárico 50	18080913	4
Caelo	Ácido esteárico 50	18238002	1
Caelo	Ácido esteárico 50	18238004	5
Caelo	Ácido esteárico 50	18238006	2
Caelo	Ácido esteárico 50	18238010	4
Caelo	Ácido esteárico 50	192910002	1
Caelo	Ácido esteárico 50	192910005	2
Caelo	Ácido esteárico 50	192910010	1
Caelo	Ácido esteárico 50	192910012	1
Caelo	Ácido esteárico 50	2000393001	1
Caelo	Ácido esteárico 50	20003933002	1
Caelo	Ácido esteárico 50	21003445001	1
Caelo	Ácido esteárico 50	21003445002	1
Caelo	Ácido esteárico 50	22000750004	4
Caelo	Ácido esteárico 50	23933002	1
Caesar & Loretz GmbH…	Ácido esteárico 50	18238010	1
Caesar & Loretz GmbH…	Ácido esteárico 50	20003933002	1
Caesar & Loretz GmbH…	Ácido esteárico 50	18238006	1
Caesar & Loretz GmbH…	Ácido esteárico 50	192910	1
Caesar & Loretz GmbH…	Ácido esteárico 50	18238006	1
Caesar & Loretz GmbH	Ácido esteárico 50	18238010	1
Caesar & Loretz GmbH	Ácido esteárico 50	192910005	5
Caesar & Loretz GmbH	Ácido esteárico 50	20003933001	3
Caesar & Loretz GmbH	Ácido esteárico 50	20003933010	1
Caesar & Loretz GmbH	Ácido esteárico 50	21003445002	1
Caesar & Loretz	Ácido esteárico 50	14359310	1
Caesar&Loretz GmbH/Anzag	Ácido esteárico 50	11308505	1
Caleo	Ácido esteárico 50	16096301	1
GEHE	Ácido esteárico 50	18238006	1
Jenne	Ácido esteárico 50	18080901	1
Kehr	Ácido esteárico 50	16346902	1
Phoenix	Ácido esteárico 50	12241915	1
Phönix	Ácido esteárico 50	1224915	1
Phönix	Ácido esteárico 50	18080901	1
ROHA	Ácido esteárico 50	130240	1

- 235 979 spectra from 1515 *Apo-Ident* customers from a total of 49 219 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ácido esteárico 50* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido esteárico 50* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	390	0	152 572
Type B	0	190	0	201 894
Type C	0	86	2	235 979

The substance/substance group *Ácido esteárico 50* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4615 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	97.7273 % (> 94.3182 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20869	20869	0,00	127,02
21793	21928	7,15	125,15
21928	21928	0,00	130,91
22274	25066	6,93	122,40
23294	23294	0,00	122,97
23667	23667	0,00	121,78
25066	25066	0,00	122,93
26125	26125	0,00	131,50

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido fólico hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20370-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido fólico hidratado; Acidum folicum hydricum

Special notes

When selecting the *Ácido fólico hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido fólico hidratado	7	6	16

Second-stage model

For differentiation of the substance/substance group *Ácido fólico hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido fólico hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	93,44	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido fólico hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido fólico hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ácido fólico hidratado	1401005-01	21288	40	20140131
Euro OTC	Ácido fólico hidratado	1508024	21891	60	20150902*
Euro OTC	Ácido fólico hidratado	1604036	22554	40	20160429*
Euro OTC	Ácido fólico hidratado	1611009	22868	40	20161201*
Euro OTC	Ácido fólico hidratado	1911019	25072	40	20191216*
Fagron	Ácido fólico hidratado	12G17-N05	20767	40	20120727
Fagron	Ácido fólico hidratado	16C03-B06-322513	23081	40	20160411

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Ácido fólico hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 9 reference samples from the substance/substance group *Ácido fólico hidratado*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido fólico hidratado	1608030	22818	40
Euro OTC	Ácido fólico hidratado	1903033	24608	40
Euro OTC	Ácido fólico hidratado	2006021	25272	40
Euro OTC	Ácido fólico hidratado	2201042	25964	40
Euro OTC	Ácido fólico hidratado	2312005	27196	40
Euro OTC	Ácido fólico hidratado	2407015	27361	40
Euro OTC	Ácido fólico hidratado	2201042	25964SI	10
Euro OTC	Ácido fólico hidratado	2312005	27196SI	20
Euro OTC	Ácido fólico hidratado	2407015	27361SI	20

- 201 794 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 20 *Apo-Ident* customers from 17 batches from the substance/substance group *Ácido fólico hidratado*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
EuRho	Ácido fólico hidratado	1911019-01	1
Euro OTC	Ácido fólico hidratado	1307041-01	1
Euro OTC	Ácido fólico hidratado	1401005-01	1
Euro OTC	Ácido fólico hidratado	1604036-01	1
Euro OTC	Ácido fólico hidratado	1608030-01	1
Euro OTC	Ácido fólico hidratado	1611009-01	5
Euro OTC	Ácido fólico hidratado	1611009-02	1
Euro OTC	Ácido fólico hidratado	1611009-04	1
Euro OTC	Ácido fólico hidratado	1903033-01	2
Euro OTC	Ácido fólico hidratado	1911019-01	2
Euro OTC	Ácido fólico hidratado	2006021-01	1
Euro OTC	Ácido fólico hidratado	2201042-01	1
Fagron	Ácido fólico hidratado	13A11-N01	1
Fagron	Ácido fólico hidratado	13G16-N02	4
Fagron	Ácido fólico hidratado	14H05-B03	1
Fagron	Ácido fólico hidratado	16C03-B06	1
Fagron	Ácido fólico hidratado	UT11110182	1
Farmalabor	Ácido fólico hidratado	P1701610	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido fólico hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido fólico hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	290	0	201 794
Type C	0	27	0	236 040

The substance/substance group *Ácido fólico hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20767	22554	4,69	116,74
21288	22554	4,54	115,98
21891	21891	0,00	113,77
22554	22554	0,00	113,72
22868	22868	0,00	113,22
23081	22554	4,51	111,08
25072	25072	0,00	115,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido fusídico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20780-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido fusídico; Acidum fusidicum

Special notes

When selecting the *Ácido fusídico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido fusídico	5	3	37

Second-stage model

For differentiation of the substance/substance group *Ácido fusídico* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido fusídico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	91,90	–
⋮	⋮	⋮
Povidona	>50	78,18
Iodopovidona	>50	89,05
Progesterona	>50	115,66
Espironolactona	>50	122,16
Propionato de testosterona	>50	176,82
Ubidecarenona	>50	223,28

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido fusídico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido fusídico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ácido fusídico	12G04-N01	20780	40	1401162
Fagron	Ácido fusídico	13L13-B01-289513	21733	60	20140113
Fagron	Ácido fusídico	14E01-B08-299791	21897	60	20140605
Fagron	Ácido fusídico	20J21-F02-375395	25493	40	2104173
Fagron	Ácido fusídico	23K21-B01-233624	27045	40	20231206

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 240 spectra of 5 reference samples from the substance/substance group *Ácido fusídico*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 722 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Ácido fusídico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ácido fusídico	15I10-B02-322112	23069	40
Fagron	Ácido fusídico	17J06-B02-343675	23943	40
Fagron	Ácido fusídico	22E23-B03-220268	26296	40
Fagron	Ácido fusídico	22E23-B03-220268	26296SI	20
Fagron	Ácido fusídico	23K21-B01-233624	27045SI†	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 55 spectra from 25 *Apo-Ident* customers from 40 batches from the substance/substance group *Ácido fusídico*.

- Among them are spectra of independent samples from 37 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Ácido fusídico	21K17-B02-216070	1
	Ácido fusídico	22E23-B03-220268	1
Caelo	Ácido fusídico	21E12-F08-378510	1
Ebert 24.08.16	Ácido fusídico	1510-B02_319452	1
Fagron	Ácido fusídico	1119I-03682	1
Fagron	Ácido fusídico	116E-03682	1
Fagron	Ácido fusídico	12B23-N03	1
Fagron	Ácido fusídico	12G04-No1	1
Fagron	Ácido fusídico	13A07-N10	2
Fagron	Ácido fusídico	13H19-N05	1
Fagron	Ácido fusídico	13L13-B01	1
Fagron	Ácido fusídico	13L13-B01-289513	3
Fagron	Ácido fusídico	13L13-B01-289514	1
Fagron	Ácido fusídico	14E01-B08-299791	3
Fagron	Ácido fusídico	15/10-b02	2
Fagron	Ácido fusídico	15/10-B02-314192	1
Fagron	Ácido fusídico	15/10-B02-319452	1
Fagron	Ácido fusídico	1510-B02_319231	1
Fagron	Ácido fusídico	15I10-B02	1
Fagron	Ácido fusídico	15I10B02-319231	1
Fagron	Ácido fusídico	15I10-B02-326182	1
Fagron	Ácido fusídico	17G06-B99-337953	1
Fagron	Ácido fusídico	17J06-B02-343677	1
Fagron	Ácido fusídico	17J06-B02-345542	1
Fagron	Ácido fusídico	17J06-B02-345885	1
Fagron	Ácido fusídico	17J06-B02-355108	1
Fagron	Ácido fusídico	20J21-F01-375395	1
Fagron	Ácido fusídico	20J21-F02-375395	1
Fagron	Ácido fusídico	20J21-F02-375397	2
Fagron	Ácido fusídico	21D12-B08-213764	2
Fagron	Ácido fusídico	21E12-F08	1
Fagron	Ácido fusídico	21E12-F08-378510	2
Fagron	Ácido fusídico	21H13-B05-213845	3
Fagron	Ácido fusídico	21H13-BO5-213845	1
Fagron	Ácido fusídico	21K17-B02-216069	3
Fagron	Ácido fusídico	318A-03682	1
Fagron	Ácido fusídico	4113U-07034	1
Fagron	Ácido fusídico	FS655	1
Noweda	Ácido fusídico	17J06-B02-349947	1
Phoenix/Cealo	Ácido fusídico	701714-0003/0918A-07	1
Phönix	Ácido fusídico	F03-3691901	1
Tagron	Ácido fusídico	17J06-B02-355108	1

- 236 012 spectra from 1515 *Apo-Ident* customers from a total of 49 218 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido fusídico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido fusídico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	160	0	201 924
Type C	0	55	0	236 012

The substance/substance group *Ácido fusídico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 89.0909 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20780	20780	0,00	121,17
21733	20780	7,12	123,10
21897	20780	32,12	121,21
25493	25493	0,00	126,48
27045	20780	32,46	133,95

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido glutâmico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20436-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido glutâmico; Acidum glutaminicum

Special notes

When selecting the *Ácido glutâmico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido glutâmico	5	2	3

Second-stage model

For differentiation of the substance/substance group *Ácido glutâmico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido glutâmico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	89,29	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido glutâmico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido glutâmico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ácido glutâmico	1604056	22562	40	20160523*
Euro OTC	Ácido glutâmico	1604056	24124	40	20180613*
Euro OTC	Ácido glutâmico	2002044	25158	40	20200513*
Euro OTC	Ácido glutâmico	2305025	26753	40	20230705*
Fagron	Ácido glutâmico	11I30-N02	20840	40	AR-15-FG-010446-02
Fagron	Ácido glutâmico	15G31-B08-311884	23599	40	20150817

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 240 spectra of 6 reference samples from the substance/substance group *Ácido glutâmico*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 722 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 3 reference samples from the substance/substance group *Ácido glutâmico*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido glutâmico	1907031	24788	40
Euro OTC	Ácido glutâmico	2008026	25405	40
Euro OTC	Ácido glutâmico	2305025	26753SI†	20

- 201 984 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Ácido glutâmico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Ácido glutâmico	2008026-01	1
Euro OTC	Ácido glutâmico	28071505	1
Fagron	Ácido glutâmico	3031502	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido glutâmico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido glutâmico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	100	0	201 984
Type C	0	3	0	236 064

The substance/substance group *Ácido glutâmico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20840	20840	0,00	157,89
22562	22562	0,00	158,85
23599	22562	7,72	125,89
24124	24124	0,00	150,07
25158	25158	0,00	158,22
26753	26753	0,00	162,78

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido nicotínico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20383-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido nicotínico; Acidum nicotinicum; Niacina

Special notes

When selecting the *Ácido nicotínico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido nicotínico	4	3	3

Second-stage model

For differentiation of the substance/substance group *Ácido nicotínico* the following second-stage model is used:

- Submodelo 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido nicotínico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	132,41	–
⋮	⋮	⋮
Mesalazina	>50	23,56
Clioquinol	>50	50,27
Nitrato de miconazol	>50	60,84
Teofilina etilenodiamina hidratada	>50	214,38

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido nicotínico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido nicotínico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ácido nicotínico	1906026	24805	40	20190711*
Fagron	Ácido nicotínico	14E01-B09-293947	21692	60	AR-15-FG-008938-01
Fagron	Ácido nicotínico	16H19-B02-330121	23225	40	AR-17-FG-016013-01
Fagron	Ácido nicotínico	21C04-B03-215782	27042	40	20210514

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Ácido nicotínico*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 782 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Ácido nicotínico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido nicotínico	1801021	23954	40
Fagron	Ácido nicotínico	18B15-B07-350570	24592	40
Fagron	Ácido nicotínico	23A11-B03-229438	26819	40
Fagron	Ácido nicotínico	23A11-B03-229438	26819SI	20
Fagron	Ácido nicotínico	21C04-B03-215782	27042SI†	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Ácido nicotínico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Euro OTC	Ácido nicotínico	1801021-01	2
Fagron	Ácido nicotínico	L17120080	1
gonmisol	Ácido nicotínico	17-18/NCN(P)/B/008	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido nicotínico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido nicotínico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	160	0	201 924
Type C	0	4	0	236 063

The substance/substance group *Ácido nicotínico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21692	21692	0,00	169,44
23225	23225	0,00	166,01
24805	24805	0,00	174,64
27042	23225	7,05	165,84

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido oxálico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20458-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido oxálico; Acidum oxalicum cryst.

Special notes

When selecting the *Ácido oxálico* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido oxálico	6	3	27

Second-stage model

For differentiation of the substance/substance group *Ácido oxálico* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido oxálico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	84,13	–
⋮	⋮	⋮
Sulfato de colistina	>50	55,21
Sulfato de polimixina B	>50	59,25
Riboflavina	>50	70,18
Bacitracina	>50	71,18
Anfotericina B	>50	81,56
Cianocobalamina	>50	86,50
Tosilcloramida sódica	>50	104,79
Carmelose sódica	>50	108,94
SyrSpend® SF pH4 neo	>50	112,56
Glicerofosfato de cálcio	>50	113,60
SyrSpend® SF Alka	>50	126,03
Bromidrato de hioscina	>50	129,75
Nistatina	>50	135,73
Triancinolona	>50	137,82
Pantotenato de cálcio	>50	141,98
Gelatina, branca	>50	144,99
Amido de trigo	>50	149,53
Estriol	>50	162,26
Amido de arroz	>50	163,41
Estradiol hemi-hidratado	>50	169,63
Frutose	>50	172,39
Levedura de selênio	>50	185,01
SyrSpend® SF pH4	>50	189,42
Goma arábica, dispersão seca	>50	193,41
Vitamina E acetato pó 50%	>50	226,70
Fécula de batata	>50	228,37
Amido de milho	>50	240,79
Maltodextrina	>50	260,04
Metilcobalamina	>50	291,76

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido oxálico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido oxálico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido oxálico	13353901	21042	40	20131029
Caelo	Ácido oxálico	12212410	21066	40	1403223
Caelo	Ácido oxálico	13353918	21774	60	20131029
Caelo	Ácido oxálico	171140	23287	40	20170426*
Caelo	Ácido oxálico	171140	23688	40	20170426*
Caelo	Ácido oxálico	18202403	24428	40	1905160
Caelo	Ácido oxálico	20000475	25207	40	20200313*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Ácido oxálico*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 662 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 4 reference samples from the substance/substance group *Ácido oxálico*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido oxálico	13353905	21453	60
Caelo	Ácido oxálico	20003046	25623	40
Caelo	Ácido oxálico	21004224	26007	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido oxálico	21004224	26007SI	10

- 201 934 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 33 spectra from 27 *Apo-Ident* customers from 29 batches from the substance/substance group *Ácido oxálico*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Ácido oxálico	10383104	1
Caelo	Ácido oxálico	11111703	1
Caelo	Ácido oxálico	12147010	1
Caelo	Ácido oxálico	12212406	1
Caelo	Ácido oxálico	12212407	1
Caelo	Ácido oxálico	12212411	1
Caelo	Ácido oxálico	13195413	1
Caelo	Ácido oxálico	13195414	1
Caelo	Ácido oxálico	13353901	1
Caelo	Ácido oxálico	13353905	3
Caelo	Ácido oxálico	13353907	2
Caelo	Ácido oxálico	13353910	1
Caelo	Ácido oxálico	13353915	1
Caelo	Ácido oxálico	14334703	1
Caelo	Ácido oxálico	15399901	1
Caelo	Ácido oxálico	16050205	1
Caelo	Ácido oxálico	16297401	1
Caelo	Ácido oxálico	17114003	1
Caelo	Ácido oxálico	17344503	1
Caelo	Ácido oxálico	18196401	1
Caelo	Ácido oxálico	4812U-01039	1
Caelo	Ácido oxálico	7111808	1
Caelo	Ácido oxálico	914E-01039	1
Caelo	Ácido oxálico	Retest17111401	2
Caesar & Loretz GmbH...	Ácido oxálico	20003046001	1
Caesar & Loretz GmbH	Ácido oxálico	20000475004	1
Caesar&Loretz GmbH/ ...	Ácido oxálico	13353920	1
Nachprüfung	Ácido oxálico		1
sanacorp	Ácido oxálico	11098213	1

- 236 034 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ácido oxálico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido oxálico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	150	0	201 934
Type C	0	33	0	236 034

The substance/substance group *Ácido oxálico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.8182 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21042	21066	6,15	147,35
21066	21066	0,00	141,74
21774	21066	7,08	141,30
23287	23287	0,00	144,73
23688	23688	0,00	144,86
24428	24428	0,00	145,91
25207	25207	0,00	132,15

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido salicílico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20015-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido salicílico; Acidum salicylicum

Special notes

When selecting the *Ácido salicílico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido salicílico	9	23	577

Second-stage model

For differentiation of the substance/substance group *Ácido salicílico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido salicílico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	136,91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido salicílico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido salicílico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido salicílico	13344002	21436	60	20131029
Caelo	Ácido salicílico	13344018	21760	60	20131020
Caelo	Ácido salicílico	160109	22443	60	20160229*
Caelo	Ácido salicílico	22001526	26113	40	20220516*
Caelo	Ácido salicílico	22001526	26113SI	20	20220516*
Euro OTC	Ácido salicílico	1110020-01	20696	40	20120125
Euro OTC	Ácido salicílico	1509007	21906	60	20150929*
Euro OTC	Ácido salicílico	2101028	25543	40	20210304*
Fagron	Ácido salicílico	16I15-B08-333932	23592	40	20170210
Fagron	Ácido salicílico	190263	24591	40	20190121

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Ácido salicílico*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 502 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1120 spectra of 31 reference samples from the substance/substance group *Ácido salicílico*.

- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido salicílico	160500	22448	60
Caelo	Ácido salicílico	171333	23277	40
Caelo	Ácido salicílico	173015	23827	40
Caelo	Ácido salicílico	182300	24236	40
Caelo	Ácido salicílico	192209	24883	40
Caelo	Ácido salicílico	21003008	25857	50
Caelo	Ácido salicílico	22001524	26103	40
Caelo	Ácido salicílico	22001528	26104	40
Caelo	Ácido salicílico	22001529	26105	40
Caelo	Ácido salicílico	22001534	26106	40
Caelo	Ácido salicílico	24000004	27235	40
Euro OTC	Ácido salicílico	1605023	22685	40
Euro OTC	Ácido salicílico	1707009	23556	40
Euro OTC	Ácido salicílico	1801042	23968	40
Euro OTC	Ácido salicílico	1901015	24471	40
Euro OTC	Ácido salicílico	1910018	24925	40
Euro OTC	Ácido salicílico	2108024	25821	50
Euro OTC	Ácido salicílico	2201044	25950	40
Euro OTC	Ácido salicílico	2208003	26280	40
Euro OTC	Ácido salicílico	2308012	26872	40
Euro OTC	Ácido salicílico	2311012	27154	40
Euro OTC	Ácido salicílico	2407001	27290	40
Fagron	Ácido salicílico	22E12-B05-227887	26609	40
Caelo	Ácido salicílico	21003008	25857SI	10
Caelo	Ácido salicílico	22001524	26103SI	20
Caelo	Ácido salicílico	22001528	26104SI	20
Caelo	Ácido salicílico	22001529	26105SI	20
Caelo	Ácido salicílico	22001534	26106SI	20
Euro OTC	Ácido salicílico	2108024	25821SI	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido salicílico	2201044	25950SI	40
Euro OTC	Ácido salicílico	2208003	26280SI	20

- 200 964 spectra from a total of 4022 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4307 spectra from 1237 *Apo-Ident* customers from 598 batches from the substance/substance group *Ácido salicílico*.
- Among them are spectra of independent samples from 572 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido salicílico	20003823016	3
	Ácido salicílico	20004424015	2
	Ácido salicílico	21003008003	1
	Ácido salicílico	21003008015	1
	Ácido salicílico	21003008016	10
	Ácido salicílico	21003008017	1
	Ácido salicílico	2100300816	1
	Ácido salicílico	2101028-01	1
	Ácido salicílico	22001528001	1
	Ácido salicílico	22001528002	4
	Ácido salicílico	22001528003	2
	Ácido salicílico	2200152802	1
	Ácido salicílico	22001529002	18
	Ácido salicílico	22001529003	2
	Ácido salicílico	220015298002	1
	Ácido salicílico	22001534003	12
	Ácido salicílico	22001534004	3
	Ácido salicílico	22001534007	1
	Ácido salicílico	2200159002	1
	Ácido salicílico	2201044-2	1
	Ácido salicílico	2208003-01	4
	Ácido salicílico	2208003-02	9
	Ácido salicílico	22D07-B03-221811	1
	Ácido salicílico	22DS07-B03-221811	1
	Ácido salicílico	22j26-b06-227888	1
	Ácido salicílico	22J26-B06-227888	1
	Ácido salicílico	22J26-B06-2278888	1
	Ácido salicílico	23002014002	1
	Ácido salicílico	23002014003	12
	Ácido salicílico	2308012-01	4
	Ácido salicílico	2311012-01	1
	Ácido salicílico	2388012-01	1
	Ácido salicílico	23B01-B01-232363	1
	Ácido salicílico	24000043001	6
	Ácido salicílico	B03-2218101	1
14076202	Ácido salicílico		1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
ACM	Ácido salicílico	KNC0461J15	1
AHC	Ácido salicílico	20004424011	1
AHC	Ácido salicílico	22001529002	1
AHD 22.07.14	Ácido salicílico	134002	1
AHD	Ácido salicílico	13344002	1
AHD	Ácido salicílico	1509007-01	1
AHD	Ácido salicílico	192209003	1
AHD	Ácido salicílico	22001524003	1
AHD	Ácido salicílico	22001528002	2
AHD	Ácido salicílico	22001529003	1
AHD	Ácido salicílico	22001534007	1
Alliance 19.12.12	Ácido salicílico	11311906	1
Alliance Healthcare	Ácido salicílico	12036215	2
Alliance Healthcare	Ácido salicílico	12036216	1
Alliance Healthcare	Ácido salicílico	15211808	1
Alliance	Ácido salicílico	21003008016	1
Anzag/Anzag 11.09.18	Ácido salicílico	18F05-B02-350586	1
Anzag/Henry Lamotte	Ácido salicílico	1334018	1
Anzag	Ácido salicílico	1303020-01	2
Anzag	Ácido salicílico	16050014	1
apo ident	Ácido salicílico	1605023-01	1
apomix	Ácido salicílico	2108024-01	1
Bombastus	Ácido salicílico	12036223	1
Bombastus	Ácido salicílico	12323403	1
Bombastus	Ácido salicílico	14L02-B02-303557	1
Bombastus	Ácido salicílico	16050017	1
Bombastus	Ácido salicílico	1605023-01	1
Bombastus	Ácido salicílico	17301505	1
Caaelo	Ácido salicílico	14336911	1
Caela	Ácido salicílico	16312001	1
Caelo	Ácido salicílico		8
Caelo	Ácido salicílico	10001612	1
Caelo	Ácido salicílico	10112014B	1
Caelo	Ácido salicílico	102455-0001	1
Caelo	Ácido salicílico	10291803	1
Caelo	Ácido salicílico	10291817	1
Caelo	Ácido salicílico	10355907	1
Caelo	Ácido salicílico	10355911	2
Caelo	Ácido salicílico	10355912	1
Caelo	Ácido salicílico	10355916	1
Caelo	Ácido salicílico	1045	1
Caelo	Ácido salicílico	11197103	1
Caelo	Ácido salicílico	11197106	1
Caelo	Ácido salicílico	11197117	1
Caelo	Ácido salicílico	11197118	1
Caelo	Ácido salicílico	11197123	4
Caelo	Ácido salicílico	11311902	2
Caelo	Ácido salicílico	11311903	1
Caelo	Ácido salicílico	11311905	1
Caelo	Ácido salicílico	11311906	2
Caelo	Ácido salicílico	11311910	2
Caelo	Ácido salicílico	11311917	4
Caelo	Ácido salicílico	11311922	9
Caelo	Ácido salicílico	11311923	2
Caelo	Ácido salicílico	117027-2	1
Caelo	Ácido salicílico	12036202	3
Caelo	Ácido salicílico	12036208	1
Caelo	Ácido salicílico	12036209	4
Caelo	Ácido salicílico	12036210	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido salicílico	12036211	3
Caelo	Ácido salicílico	12036215	2
Caelo	Ácido salicílico	12036216	5
Caelo	Ácido salicílico	12036217	2
Caelo	Ácido salicílico	12036223	8
Caelo	Ácido salicílico	12036225	4
Caelo	Ácido salicílico	12036226	7
Caelo	Ácido salicílico	12036315	1
Caelo	Ácido salicílico	12134702	12
Caelo	Ácido salicílico	12134707	6
Caelo	Ácido salicílico	12134709	23
Caelo	Ácido salicílico	12134710	1
Caelo	Ácido salicílico	12134711	10
Caelo	Ácido salicílico	12134712	4
Caelo	Ácido salicílico	12134713	1
Caelo	Ácido salicílico	12134714	16
Caelo	Ácido salicílico	12134715	7
Caelo	Ácido salicílico	12134717	9
Caelo	Ácido salicílico	12134719	4
Caelo	Ácido salicílico	12134720	8
Caelo	Ácido salicílico	12134721	2
Caelo	Ácido salicílico	12134722	4
Caelo	Ácido salicílico	123134712	1
Caelo	Ácido salicílico	12323401	1
Caelo	Ácido salicílico	12323402	2
Caelo	Ácido salicílico	12323403	3
Caelo	Ácido salicílico	1234	1
Caelo	Ácido salicílico	1234709	1
Caelo	Ácido salicílico	12374204	1
Caelo	Ácido salicílico	12374205	8
Caelo	Ácido salicílico	12374207	6
Caelo	Ácido salicílico	12374207-3454311172	1
Caelo	Ácido salicílico	12374208	2
Caelo	Ácido salicílico	12374210	3
Caelo	Ácido salicílico	12374211	18
Caelo	Ácido salicílico	12374212	2
Caelo	Ácido salicílico	12374213	11
Caelo	Ácido salicílico	1274210	1
Caelo	Ácido salicílico	12H10-N08	5
Caelo	Ácido salicílico	1303020-01	2
Caelo	Ácido salicílico	13032014A	1
Caelo	Ácido salicílico	13101707	1
Caelo	Ácido salicílico	1310516	1
Caelo	Ácido salicílico	13344002	20
Caelo	Ácido salicílico	13344003	10
Caelo	Ácido salicílico	13344013	11
Caelo	Ácido salicílico	13344014	6
Caelo	Ácido salicílico	13344018	19
Caelo	Ácido salicílico	13344020	17
Caelo	Ácido salicílico	1334403	1
Caelo	Ácido salicílico	133454002	1
Caelo	Ácido salicílico	13B14-No1	1
Caelo	Ácido salicílico	13H01-N01	1
Caelo	Ácido salicílico	13H01-N04	2
Caelo	Ácido salicílico	1406027	1
Caelo	Ácido salicílico	140602701	1
Caelo	Ácido salicílico	1406027-02	3
Caelo	Ácido salicílico	14076201	1
Caelo	Ácido salicílico	14076202	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido salicílico	14076203	7
Caelo	Ácido salicílico	14076204	11
Caelo	Ácido salicílico	14076206	7
Caelo	Ácido salicílico	14076207	10
Caelo	Ácido salicílico	14076211	1
Caelo	Ácido salicílico	14076212	1
Caelo	Ácido salicílico	14300801	8
Caelo	Ácido salicílico	14300802	6
Caelo	Ácido salicílico	14300804	7
Caelo	Ácido salicílico	14300805	11
Caelo	Ácido salicílico	14300806	1
Caelo	Ácido salicílico	14300808	1
Caelo	Ácido salicílico	14300809	12
Caelo	Ácido salicílico	1430802	1
Caelo	Ácido salicílico	1433620	1
Caelo	Ácido salicílico	14336904	2
Caelo	Ácido salicílico	14336905	15
Caelo	Ácido salicílico	14336906	4
Caelo	Ácido salicílico	14336907	26
Caelo	Ácido salicílico	14336908	3
Caelo	Ácido salicílico	14336911	24
Caelo	Ácido salicílico	14336912	9
Caelo	Ácido salicílico	14336919	24
Caelo	Ácido salicílico	14336920	24
Caelo	Ácido salicílico	14336921	1
Caelo	Ácido salicílico	14E26-B04-294622	1
Caelo	Ácido salicílico	14L02-B02-303558	1
Caelo	Ácido salicílico	15081601	1
Caelo	Ácido salicílico	15084401	4
Caelo	Ácido salicílico	15084403	7
Caelo	Ácido salicílico	15084404	3
Caelo	Ácido salicílico	1509007-01	1
Caelo	Ácido salicílico	1509007-02	2
Caelo	Ácido salicílico	151224/1	1
Caelo	Ácido salicílico	152117304	1
Caelo	Ácido salicílico	15211803	1
Caelo	Ácido salicílico	15211806	2
Caelo	Ácido salicílico	15211807	2
Caelo	Ácido salicílico	15211808	10
Caelo	Ácido salicílico	15211809	14
Caelo	Ácido salicílico	15211810	10
Caelo	Ácido salicílico	15217301	6
Caelo	Ácido salicílico	15217302	19
Caelo	Ácido salicílico	15217303	9
Caelo	Ácido salicílico	15217304	7
Caelo	Ácido salicílico	15217305	6
Caelo	Ácido salicílico	15217308	8
Caelo	Ácido salicílico	15217309	1
Caelo	Ácido salicílico	16/15-B08-332098	1
Caelo	Ácido salicílico	1600917	1
Caelo	Ácido salicílico	16010901	5
Caelo	Ácido salicílico	16010901s	1
Caelo	Ácido salicílico	16010903	17
Caelo	Ácido salicílico	16010904	12
Caelo	Ácido salicílico	16010905	11
Caelo	Ácido salicílico	16010906	17
Caelo	Ácido salicílico	16010907	6
Caelo	Ácido salicílico	16010908	3
Caelo	Ácido salicílico	16010910	17

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido salicílico	16010911	4
Caelo	Ácido salicílico	16010912	4
Caelo	Ácido salicílico	160109123	1
Caelo	Ácido salicílico	16010913	18
Caelo	Ácido salicílico	16010916	5
Caelo	Ácido salicílico	16010917	16
Caelo	Ácido salicílico	16010918	11
Caelo	Ácido salicílico	16010921	3
Caelo	Ácido salicílico	16010922	16
Caelo	Ácido salicílico	16010923	7
Caelo	Ácido salicílico	16010972	1
Caelo	Ácido salicílico	1601916	1
Caelo	Ácido salicílico	160405AS	1
Caelo	Ácido salicílico	160500004	3
Caelo	Ácido salicílico	16050003	2
Caelo	Ácido salicílico	16050004	18
Caelo	Ácido salicílico	16050005	11
Caelo	Ácido salicílico	16050006	3
Caelo	Ácido salicílico	16050011	15
Caelo	Ácido salicílico	16050012	16
Caelo	Ácido salicílico	16050013	26
Caelo	Ácido salicílico	16050014	30
Caelo	Ácido salicílico	16050016	1
Caelo	Ácido salicílico	16050017	18
Caelo	Ácido salicílico	1605023-01	1
Caelo	Ácido salicílico	1605023-02	2
Caelo	Ácido salicílico	16072014A	1
Caelo	Ácido salicílico	163120	1
Caelo	Ácido salicílico	16312001	24
Caelo	Ácido salicílico	16312003	12
Caelo	Ácido salicílico	16312004	2
Caelo	Ácido salicílico	16312005	30
Caelo	Ácido salicílico	16312008	1
Caelo	Ácido salicílico	16312009	13
Caelo	Ácido salicílico	16312010	25
Caelo	Ácido salicílico	16312012	4
Caelo	Ácido salicílico	16E02-B09-325355	1
Caelo	Ácido salicílico	16I15-B08	1
Caelo	Ácido salicílico	16i15-B08-0001	1
Caelo	Ácido salicílico	170301506	1
Caelo	Ácido salicílico	170509AS/16050012	1
Caelo	Ácido salicílico	17051803	1
Caelo	Ácido salicílico	1707009-01	4
Caelo	Ácido salicílico	170700902	1
Caelo	Ácido salicílico	17123301	1
Caelo	Ácido salicílico	1713301	1
Caelo	Ácido salicílico	1713307	1
Caelo	Ácido salicílico	17133301	26
Caelo	Ácido salicílico	17133303	23
Caelo	Ácido salicílico	17133304	4
Caelo	Ácido salicílico	17133307	59
Caelo	Ácido salicílico	171333207	1
Caelo	Ácido salicílico	1714Q1045	1
Caelo	Ácido salicílico	17301502	25
Caelo	Ácido salicílico	17301503	28
Caelo	Ácido salicílico	17301504	5
Caelo	Ácido salicílico	17301505	27
Caelo	Ácido salicílico	17301506	57
Caelo	Ácido salicílico	17301507	21

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido salicílico	17301509	36
Caelo	Ácido salicílico	17301511	11
Caelo	Ácido salicílico	17301512	31
Caelo	Ácido salicílico	17301512/P-04041921	1
Caelo	Ácido salicílico	17301612	1
Caelo	Ácido salicílico	1738980	1
Caelo	Ácido salicílico	17901506	1
Caelo	Ácido salicílico	17C21-B09-337172	2
Caelo	Ácido salicílico	17C21-B09-337173	1
Caelo	Ácido salicílico	180050009	1
Caelo	Ácido salicílico	180104201	1
Caelo	Ácido salicílico	1801042-01	5
Caelo	Ácido salicílico	18050002	12
Caelo	Ácido salicílico	18050005	1
Caelo	Ácido salicílico	18050006	38
Caelo	Ácido salicílico	18050007	19
Caelo	Ácido salicílico	18050009	27
Caelo	Ácido salicílico	1805009	1
Caelo	Ácido salicílico	18121412	1
Caelo	Ácido salicílico	181473001	9
Caelo	Ácido salicílico	18147302	31
Caelo	Ácido salicílico	18147303	13
Caelo	Ácido salicílico	18147305	1
Caelo	Ácido salicílico	18147307	1
Caelo	Ácido salicílico	18147308	19
Caelo	Ácido salicílico	18147310	26
Caelo	Ácido salicílico	18147314	40
Caelo	Ácido salicílico	18147315	5
Caelo	Ácido salicílico	18147317	17
Caelo	Ácido salicílico	18147321	43
Caelo	Ácido salicílico	182300002P-200609-3	1
Caelo	Ácido salicílico	18230002	3
Caelo	Ácido salicílico	18230002P-200806-1	1
Caelo	Ácido salicílico	18230004	18
Caelo	Ácido salicílico	18230004/P-26041921	1
Caelo	Ácido salicílico	18230007	46
Caelo	Ácido salicílico	18230009	15
Caelo	Ácido salicílico	18230010	1
Caelo	Ácido salicílico	18230013	4
Caelo	Ácido salicílico	18306909	1
Caelo	Ácido salicílico	18E24-B03-354310	1
Caelo	Ácido salicílico	18E24-B03-354311	3
Caelo	Ácido salicílico	18F05-B02-352210	2
Caelo	Ácido salicílico	1901015-01	2
Caelo	Ácido salicílico	190263	2
Caelo	Ácido salicílico	190264	2
Caelo	Ácido salicílico	190312004	1
Caelo	Ácido salicílico	1906105	1
Caelo	Ácido salicílico	190612001	26
Caelo	Ácido salicílico	190612003	1
Caelo	Ácido salicílico	190612004	37
Caelo	Ácido salicílico	19061201	3
Caelo	Ácido salicílico	19061202	13
Caelo	Ácido salicílico	19061205	38
Caelo	Ácido salicílico	19061206	33
Caelo	Ácido salicílico	19062001	1
Caelo	Ácido salicílico	1906612001	1
Caelo	Ácido salicílico	1910018-01	1
Caelo	Ácido salicílico	1910018-03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido salicílico	1913Q-01045	1
Caelo	Ácido salicílico	1922090003	1
Caelo	Ácido salicílico	192209001	29
Caelo	Ácido salicílico	192209003	29
Caelo	Ácido salicílico	192209006	9
Caelo	Ácido salicílico	1961206	1
Caelo	Ácido salicílico	200000147004	1
Caelo	Ácido salicílico	20000146005	13
Caelo	Ácido salicílico	20000147002	25
Caelo	Ácido salicílico	20000147002/4720	1
Caelo	Ácido salicílico	20000147004	27
Caelo	Ácido salicílico	20000147006	20
Caelo	Ácido salicílico	200004424004	1
Caelo	Ácido salicílico	200004424012	1
Caelo	Ácido salicílico	20003823008	31
Caelo	Ácido salicílico	20003823010	7
Caelo	Ácido salicílico	20003823011	2
Caelo	Ácido salicílico	20003823014	5
Caelo	Ácido salicílico	20003823015	1
Caelo	Ácido salicílico	20003823016	10
Caelo	Ácido salicílico	2000442004	1
Caelo	Ácido salicílico	20004421006	1
Caelo	Ácido salicílico	20004424001	15
Caelo	Ácido salicílico	20004424004	28
Caelo	Ácido salicílico	20004424006	27
Caelo	Ácido salicílico	20004424007	3
Caelo	Ácido salicílico	20004424009	1
Caelo	Ácido salicílico	20004424010	26
Caelo	Ácido salicílico	20004424011	8
Caelo	Ácido salicílico	20004424012	20
Caelo	Ácido salicílico	20004424015	8
Caelo	Ácido salicílico	2004424001	1
Caelo	Ácido salicílico	20111306	1
Caelo	Ácido salicílico	20151112-4	1
Caelo	Ácido salicílico	2017-11-23-AXILU	1
Caelo	Ácido salicílico	20270312-2	1
Caelo	Ácido salicílico	207102017/16050017	1
Caelo	Ácido salicílico	21000488001	14
Caelo	Ácido salicílico	21003008001	5
Caelo	Ácido salicílico	21003008003	5
Caelo	Ácido salicílico	21003008004	17
Caelo	Ácido salicílico	21003008009	8
Caelo	Ácido salicílico	21003008010	8
Caelo	Ácido salicílico	21003008015	1
Caelo	Ácido salicílico	21003008016	2
Caelo	Ácido salicílico	21003008017	1
Caelo	Ácido salicílico	2100488001	1
Caelo	Ácido salicílico	2101028-01	1
Caelo	Ácido salicílico	2103008004	1
Caelo	Ácido salicílico	216E-03750	1
Caelo	Ácido salicílico	220001524003	1
Caelo	Ácido salicílico	22001158002	1
Caelo	Ácido salicílico	22001524003	23
Caelo	Ácido salicílico	22001528001	6
Caelo	Ácido salicílico	22001528002	8
Caelo	Ácido salicílico	22001534003	2
Caelo	Ácido salicílico	23002014002	1
Caelo	Ácido salicílico	23002014003	1
Caelo	Ácido salicílico	23071510	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido salicílico	25041304	1
Caelo	Ácido salicílico	2882	1
Caelo	Ácido salicílico	31012023-01	1
Caelo	Ácido salicílico	3111J01045	1
Caelo	Ácido salicílico	3344003	1
Caelo	Ácido salicílico	3601413011-12374211	1
Caelo	Ácido salicílico	3816Q-01045	1
Caelo	Ácido salicílico	3944581	1
Caelo	Ácido salicílico	3948107	1
Caelo	Ácido salicílico	4010Q-01045	1
Caelo	Ácido salicílico	415593	1
Caelo	Ácido salicílico	4515E-01045	1
Caelo	Ácido salicílico	501171101	1
Caelo	Ácido salicílico	5112V01405	1
Caelo	Ácido salicílico	54168742	1
Caelo	Ácido salicílico	6/20151706	1
Caelo	Ácido salicílico	7071403	1
Caelo	Ácido salicílico	72(18230009)	1
Caelo	Ácido salicílico	73(20004424001)	1
Caelo	Ácido salicílico	7466	1
Caelo	Ácido salicílico	8170717	1
Caelo	Ácido salicílico	8715	1
Caelo	Ácido salicílico	9091301	1
Caelo	Ácido salicílico	9112013A	1
Caelo	Ácido salicílico	9220715	1
Caelo	Ácido salicílico	922090031	1
Caelo	Ácido salicílico	922090061	1
Caelo	Ácido salicílico	A-100513-1	1
Caelo	Ácido salicílico	A320004424007	1
Caelo	Ácido salicílico	RAS1135100	1
Caelo	Ácido salicílico	RAS1703500	1
Caelo	Ácido salicílico	test	1
Caelo	Ácido salicílico	Validierungsmessung	1
Caeo	Ácido salicílico	1010905	1
Caeolo/Alliance	Ácido salicílico	21003008010	1
Caesaer/Jenne	Ácido salicílico	18050006	1
Caesar & Loretz GmbH...	Ácido salicílico	22001524003	1
Caesar & Loretz GmbH...	Ácido salicílico	18147308	1
Caesar & Loretz GmbH...	Ácido salicílico	18147310	1
Caesar & Loretz GmbH...	Ácido salicílico	22001524003	2
Caesar & Loretz GmbH...	Ácido salicílico	17301512	1
Caesar & Loretz GmbH...	Ácido salicílico	18050006	2
Caesar & Loretz GmbH...	Ácido salicílico	20000147004	1
Caesar & Loretz GmbH...	Ácido salicílico	20003823016	1
Caesar & Loretz GmbH...	Ácido salicílico	18147321	1
Caesar & Loretz GmbH...	Ácido salicílico	18147314	3
Caesar & Loretz GmbH...	Ácido salicílico	190612004	1
Caesar & Loretz GmbH...	Ácido salicílico	19061206	1
Caesar & Loretz GmbH...	Ácido salicílico	11311904	1
Caesar & Loretz GmbH...	Ácido salicílico	12134714	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424001	1
Caesar & Loretz GmbH...	Ácido salicílico	11311917	1
Caesar & Loretz GmbH/ AHD	Ácido salicílico	18230004	1
Caesar & Loretz GmbH...	Ácido salicílico	192209001	1
Caesar & Loretz GmbH...	Ácido salicílico	190612004	1
Caesar & Loretz GmbH...	Ácido salicílico	18147314	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424011	1
Caesar & Loretz GmbH...	Ácido salicílico	18147314	1
Caesar & Loretz GmbH/AEP	Ácido salicílico	18230009	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/AHD	Ácido salicílico	18147321	1
Caesar & Loretz GmbH/AHD	Ácido salicílico	20004424004	1
Caesar & Loretz GmbH/AHD	Ácido salicílico	21003008004	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424004	3
Caesar & Loretz GmbH...	Ácido salicílico	18050006	1
Caesar & Loretz GmbH/G	Ácido salicílico	20004424004	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	18147308	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	192209001	1
Caesar & Loretz GmbH/GEHE	Ácido salicílico	192209006	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	20000146	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	20003823008	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	20003823014	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	20004424006	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	20004424011	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	21000488001	2
Caesar & Loretz GmbH/Gehe	Ácido salicílico	21003008001	1
Caesar & Loretz GmbH/Gehe	Ácido salicílico	22001528001	1
Caesar & Loretz GmbH...	Ácido salicílico	192209001	2
Caesar & Loretz GmbH...	Ácido salicílico	20004424010	2
Caesar & Loretz GmbH...	Ácido salicílico	22001528002	2
Caesar & Loretz GmbH/Gö	Ácido salicílico	18147321	1
Caesar & Loretz GmbH...	Ácido salicílico	18147314	1
Caesar & Loretz GmbH...	Ácido salicílico	20003823008	1
Caesar & Loretz GmbH...	Ácido salicílico	18147308	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424011	1
Caesar & Loretz GmbH/Kehr	Ácido salicílico	19061205	1
Caesar & Loretz GmbH/Kehr	Ácido salicílico	192209006	1
Caesar & Loretz GmbH/Kehr	Ácido salicílico	2100308015	1
Caesar & Loretz GmbH/Now.	Ácido salicílico	18147321	1
Caesar & Loretz GmbH...	Ácido salicílico	190612004	1
Caesar & Loretz GmbH...	Ácido salicílico	19061206	1
Caesar & Loretz GmbH...	Ácido salicílico	192209003	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424004	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424015	1
Caesar & Loretz GmbH/Otto	Ácido salicílico	19061202	1
Caesar & Loretz GmbH...	Ácido salicílico	22001524003	1
Caesar & Loretz GmbH...	Ácido salicílico	22001528002	2
Caesar & Loretz GmbH...	Ácido salicílico	18147321	2
Caesar & Loretz GmbH...	Ácido salicílico	18230007	1
Caesar & Loretz GmbH...	Ácido salicílico	19061206	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424001	1
Caesar & Loretz GmbH...	Ácido salicílico	20004424006	2
Caesar & Loretz GmbH...	Ácido salicílico	22001528001	2
Caesar & Loretz GmbH...	Ácido salicílico	20000146005	1
Caesar & Loretz GmbH...	Ácido salicílico	20000147002	1
Caesar & Loretz GmbH...	Ácido salicílico	20000147004	1
Caesar & Loretz GmbH...	Ácido salicílico	20000147006	1
Caesar & Loretz GmbH...	Ácido salicílico	18230009	1
Caesar & Loretz GmbH	Ácido salicílico	11311922	1
Caesar & Loretz GmbH	Ácido salicílico	13344003	1
Caesar & Loretz GmbH	Ácido salicílico	14300809	1
Caesar & Loretz GmbH	Ácido salicílico	16312001	1
Caesar & Loretz GmbH	Ácido salicílico	16312005	1
Caesar & Loretz GmbH	Ácido salicílico	16312012	1
Caesar & Loretz GmbH	Ácido salicílico	17133301	1
Caesar & Loretz GmbH	Ácido salicílico	17301509	1
Caesar & Loretz GmbH	Ácido salicílico	17301512	9
Caesar & Loretz GmbH	Ácido salicílico	18050002	1
Caesar & Loretz GmbH	Ácido salicílico	18050006	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ácido salicílico	18050007	2
Caesar & Loretz GmbH	Ácido salicílico	18050009	4
Caesar & Loretz GmbH	Ácido salicílico	18147302	9
Caesar & Loretz GmbH	Ácido salicílico	18147303	6
Caesar & Loretz GmbH	Ácido salicílico	18147308	3
Caesar & Loretz GmbH	Ácido salicílico	18147310	3
Caesar & Loretz GmbH	Ácido salicílico	18147313	1
Caesar & Loretz GmbH	Ácido salicílico	18147314	6
Caesar & Loretz GmbH	Ácido salicílico	18147315	2
Caesar & Loretz GmbH	Ácido salicílico	18147317	3
Caesar & Loretz GmbH	Ácido salicílico	18147321	17
Caesar & Loretz GmbH	Ácido salicílico	18147322	1
Caesar & Loretz GmbH	Ácido salicílico	18230004	3
Caesar & Loretz GmbH	Ácido salicílico	18230007	7
Caesar & Loretz GmbH	Ácido salicílico	18230009	3
Caesar & Loretz GmbH	Ácido salicílico	18230013	2
Caesar & Loretz GmbH	Ácido salicílico	1847302	1
Caesar & Loretz GmbH	Ácido salicílico	190612001	9
Caesar & Loretz GmbH	Ácido salicílico	190612003	1
Caesar & Loretz GmbH	Ácido salicílico	190612004	6
Caesar & Loretz GmbH	Ácido salicílico	19061201	1
Caesar & Loretz GmbH	Ácido salicílico	19061202	1
Caesar & Loretz GmbH	Ácido salicílico	19061205	12
Caesar & Loretz GmbH	Ácido salicílico	19061206	9
Caesar & Loretz GmbH	Ácido salicílico	192209001	8
Caesar & Loretz GmbH	Ácido salicílico	192209003	9
Caesar & Loretz GmbH	Ácido salicílico	192209004	2
Caesar & Loretz GmbH	Ácido salicílico	192209006	5
Caesar & Loretz GmbH	Ácido salicílico	20000146004	4
Caesar & Loretz GmbH	Ácido salicílico	20000146005	5
Caesar & Loretz GmbH	Ácido salicílico	20000147002	15
Caesar & Loretz GmbH	Ácido salicílico	20000147004	14
Caesar & Loretz GmbH	Ácido salicílico	20000147006	11
Caesar & Loretz GmbH	Ácido salicílico	2000147002	1
Caesar & Loretz GmbH	Ácido salicílico	20003823008	11
Caesar & Loretz GmbH	Ácido salicílico	20003823010	5
Caesar & Loretz GmbH	Ácido salicílico	20003823011	1
Caesar & Loretz GmbH	Ácido salicílico	20003823014	4
Caesar & Loretz GmbH	Ácido salicílico	20003823015	1
Caesar & Loretz GmbH	Ácido salicílico	20003823016	3
Caesar & Loretz GmbH	Ácido salicílico	20004424001	7
Caesar & Loretz GmbH	Ácido salicílico	20004424002	2
Caesar & Loretz GmbH	Ácido salicílico	20004424004	5
Caesar & Loretz GmbH	Ácido salicílico	20004424006	4
Caesar & Loretz GmbH	Ácido salicílico	20004424007	4
Caesar & Loretz GmbH	Ácido salicílico	20004424009	1
Caesar & Loretz GmbH	Ácido salicílico	20004424010	5
Caesar & Loretz GmbH	Ácido salicílico	20004424011	2
Caesar & Loretz GmbH	Ácido salicílico	20004424012	3
Caesar & Loretz GmbH	Ácido salicílico	20004424013	4
Caesar & Loretz GmbH	Ácido salicílico	20004424015	2
Caesar & Loretz GmbH	Ácido salicílico	21003008001	4
Caesar & Loretz GmbH	Ácido salicílico	21003008003	5
Caesar & Loretz GmbH	Ácido salicílico	21003008004	15
Caesar & Loretz GmbH	Ácido salicílico	21003008009	3
Caesar & Loretz GmbH	Ácido salicílico	21003008010	7
Caesar & Loretz GmbH	Ácido salicílico	21003008015	1
Caesar & Loretz GmbH	Ácido salicílico	21003008016	2
Caesar & Loretz GmbH	Ácido salicílico	22001088004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ácido salicílico	22001524003	1
Caesar & Loretz GmbH	Ácido salicílico	22001528001	4
Caesar & Loretz GmbH	Ácido salicílico	22001528002	5
Caesar & Loretz Hild…	Ácido salicílico	192209001	1
Caesar & Loretz Hilden	Ácido salicílico	17301512	1
Caesar & Loretz Hilden	Ácido salicílico	18230007	1
Caesar & Loretz Hilden	Ácido salicílico	19061205	1
Caesar & Loretz Hilden	Ácido salicílico	192209003	1
Caesar & Loretz/Gehe	Ácido salicílico	20000147004	1
Caesar & Loretz/Geil…	Ácido salicílico	17301509	1
Caesar & Loretz/Sanacorp	Ácido salicílico	17301503	1
Caesar & Loretz	Ácido salicílico	17301502	1
Caesar & Loretz	Ácido salicílico	21003008001	1
Caesar & Loretz	Ácido salicílico	21003008009	1
Caesar / Ebert & Jacobi	Ácido salicílico	16312010	2
Caesar Loretz	Ácido salicílico	192209001	1
Caesar u. Loretz GmbH	Ácido salicílico	190612004	1
Caesar u. Loretz GmbH	Ácido salicílico	192209006	1
Caesar und Loretz GmbH	Ácido salicílico	16312003	1
Caesar&Lorenz / Gehe	Ácido salicílico	18230004	1
Caesar&Lorenz	Ácido salicílico	20004424006	1
Caesar&Loretz Anzag	Ácido salicílico	14300804	2
Caesar&Loretz GmbH,1…	Ácido salicílico	16312001	1
Caesar&Loretz GmbH/Anzag	Ácido salicílico	12374204	1
Caesar&Loretz GmbH/Anzag	Ácido salicílico	14076203	2
Caesar&Loretz GmbH/S…	Ácido salicílico	15217301	1
Caesar&Loretz GmbH/S…	Ácido salicílico	18230009	1
Caesar&loretz,Anzag	Ácido salicílico	12036211	1
Caesar&loretz,Phoenix	Ácido salicílico	11197104	1
Caesar&loretz,Phoenix	Ácido salicílico	14076212	1
Caesar&loretz,Phoenix	Ácido salicílico	9220710	1
Caesar&Loretz/AHD	Ácido salicílico	15211808	1
Caesar&Loretz	Ácido salicílico	18230007	1
caesar	Ácido salicílico	15217301	1
Caleo/n	Ácido salicílico	17301502	1
Caleo/Phoenix	Ácido salicílico	21003008003	1
Caolo- Noweda	Ácido salicílico	14300809	2
carlo	Ácido salicílico	12134714	2
Cealo/Gehe	Ácido salicílico	20000147004	1
Cealo/Noweda	Ácido salicílico	17301509	1
Cealo/Sanacorp	Ácido salicílico	17133307	1
Cealo/Sanacorp	Ácido salicílico	20000147006	1
Cealo	Ácido salicílico	15211806	1
cealo	Ácido salicílico	18050007	1
Celo/ Sanacorp	Ácido salicílico	16010908	1
Delta	Ácido salicílico	17133303	1
E Plus	Ácido salicílico	16I15-B08-333932	1
Ebert 24.08.16	Ácido salicílico	16010903	1
Ebert & Jacobi	Ácido salicílico	16010923	1
EuRho 001	Ácido salicílico	1509007-02	1
Eurho/ Noweda	Ácido salicílico	1901015-01	1
Eurho/ Noweda	Ácido salicílico	1901015-03	1
EuRho/ Phönix	Ácido salicílico	RAS1730100	1
EuRho/Gehe	Ácido salicílico	1910018-01	1
EuRho/Noweda	Ácido salicílico	1910018-02	1
Eurho/Phoenix	Ácido salicílico	13B14-N01	2
EuRho/VDL	Ácido salicílico	1801042-01	1
EuRho	Ácido salicílico		1
EuRho	Ácido salicílico	1206007-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Ácido salicílico	1303020-01	1
EuRho	Ácido salicílico	1406027-01	2
EuRho	Ácido salicílico	1406027-02	1
EuRho	Ácido salicílico	1707009-01	2
EuRho	Ácido salicílico	1801042-01	2
EuRho	Ácido salicílico	1901015-01	1
EuRho	Ácido salicílico	1910018-01	1
EuRho	Ácido salicílico	1910018-03	1
EuRho	Ácido salicílico	2101028-01	1
euro AHD	Ácido salicílico	1707009-025709	1
Euro OTC	Ácido salicílico		1
Euro OTC	Ácido salicílico	102455	1
Euro OTC	Ácido salicílico	1110020	1
Euro OTC	Ácido salicílico	1110020-01	4
Euro OTC	Ácido salicílico	115465478596	1
Euro OTC	Ácido salicílico	1206007-01	7
Euro OTC	Ácido salicílico	130302001	1
Euro OTC	Ácido salicílico	1303020-01	19
Euro OTC	Ácido salicílico	1303020-02	4
Euro OTC	Ácido salicílico	1406027-01	8
Euro OTC	Ácido salicílico	140602702	1
Euro OTC	Ácido salicílico	1406027-02	12
Euro OTC	Ácido salicílico	1406027-02Mg1kg	1
Euro OTC	Ácido salicílico	14076202	1
Euro OTC	Ácido salicílico	1408027	1
Euro OTC	Ácido salicílico	14E26-B04-294622	1
Euro OTC	Ácido salicílico	1509007/02	1
Euro OTC	Ácido salicílico	1509007-01	26
Euro OTC	Ácido salicílico	150900702	1
Euro OTC	Ácido salicílico	1509007-02	12
Euro OTC	Ácido salicílico	1511023B	1
Euro OTC	Ácido salicílico	15217301	1
Euro OTC	Ácido salicílico	16/15-B08-330773	1
Euro OTC	Ácido salicílico	16050013	1
Euro OTC	Ácido salicílico	1605023/02	1
Euro OTC	Ácido salicílico	160502301	2
Euro OTC	Ácido salicílico	1605023-01	19
Euro OTC	Ácido salicílico	160502302	1
Euro OTC	Ácido salicílico	1605023-02	23
Euro OTC	Ácido salicílico	160502331	1
Euro OTC	Ácido salicílico	16E02-B09-325356	1
Euro OTC	Ácido salicílico	1707009	1
Euro OTC	Ácido salicílico	170700901	4
Euro OTC	Ácido salicílico	1707009-01	26
Euro OTC	Ácido salicílico	170700902	1
Euro OTC	Ácido salicílico	1707009-02	14
Euro OTC	Ácido salicílico	1707009-04	2
Euro OTC	Ácido salicílico	1707009-1	1
Euro OTC	Ácido salicílico	17133307	1
Euro OTC	Ácido salicílico	17301509	1
Euro OTC	Ácido salicílico	18001042-01	1
Euro OTC	Ácido salicílico	1801042	1
Euro OTC	Ácido salicílico	180104201	10
Euro OTC	Ácido salicílico	1801042-01	54
Euro OTC	Ácido salicílico	18050007	1
Euro OTC	Ácido salicílico	19001501	1
Euro OTC	Ácido salicílico	1901015-01	25
Euro OTC	Ácido salicílico	1901015-02	14
Euro OTC	Ácido salicílico	190101503	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Ácido salicílico	1901015-03	12
Euro OTC	Ácido salicílico	1901015-04	1
Euro OTC	Ácido salicílico	1901018-03	1
Euro OTC	Ácido salicílico	1910015-01	1
Euro OTC	Ácido salicílico	191001801	2
Euro OTC	Ácido salicílico	1910018-01	36
Euro OTC	Ácido salicílico	1910018-02	9
Euro OTC	Ácido salicílico	1910018-03	7
Euro OTC	Ácido salicílico	1910018-18	1
Euro OTC	Ácido salicílico	210102801	1
Euro OTC	Ácido salicílico	2101028-01	18
Euro OTC	Ácido salicílico	2108024-01	11
Euro OTC	Ácido salicílico	2201044-01	2
Euro OTC	Ácido salicílico	2201044-02	6
Euro OTC	Ácido salicílico	2208003-01	2
Euro OTC	Ácido salicílico	2208003-02	1
Euro OTC	Ácido salicílico	ras1512800	1
Euro OTC	Ácido salicílico	RAS1703500	2
Euro OTC	Ácido salicílico	RAS1920400	1
Euro/Phönix	Ácido salicílico	1801042-01	2
Euro	Ácido salicílico	1509007-02	2
Europ Ots Pharma	Ácido salicílico	12374205	1
EurRho/ Anzag	Ácido salicílico	1509007-01	1
Fagaron	Ácido salicílico	14Lo2-B02-303558	1
Fagron	Ácido salicílico		2
Fagron	Ácido salicílico	102455-0002	1
Fagron	Ácido salicílico	11197121	1
Fagron	Ácido salicílico	1140616	1
Fagron	Ácido salicílico	11K10-N01	2
Fagron	Ácido salicílico	11L19-N21	1
Fagron	Ácido salicílico	12C20-N04	1
Fagron	Ácido salicílico	12c20n12	1
Fagron	Ácido salicílico	12C20-N12	5
Fagron	Ácido salicílico	12H10-N03	8
Fagron	Ácido salicílico	12H10-N08	3
Fagron	Ácido salicílico	13344013	1
Fagron	Ácido salicílico	13B14-N01	18
Fagron	Ácido salicílico	13H01N01	1
Fagron	Ácido salicílico	13H01-N01	6
Fagron	Ácido salicílico	13H01N04	4
Fagron	Ácido salicílico	13H01-N04	13
Fagron	Ácido salicílico	13H01-N08	2
Fagron	Ácido salicílico	13K08-B31-290852	5
Fagron	Ácido salicílico	13K08-B31-290853	6
Fagron	Ácido salicílico	14300801	1
Fagron	Ácido salicílico	14300805	1
Fagron	Ácido salicílico	14336920	1
Fagron	Ácido salicílico	14B05B30	1
Fagron	Ácido salicílico	14B05-B30	2
Fagron	Ácido salicílico	14B05-B30-290854	5
Fagron	Ácido salicílico	14E26_B04	1
Fagron	Ácido salicílico	14E26B04	1
Fagron	Ácido salicílico	14E26-B04	7
Fagron	Ácido salicílico	14E26-B04_294623	1
Fagron	Ácido salicílico	14E26-B04-294622	1
Fagron	Ácido salicílico	14e26-b04-294623	1
Fagron	Ácido salicílico	14e26-B04-294623	1
Fagron	Ácido salicílico	14E26B04294623	1
Fagron	Ácido salicílico	14E26-B04-294623	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ácido salicílico	14E26-B04-294624	7
Fagron	Ácido salicílico	14E26-B04-296424	1
Fagron	Ácido salicílico	14L02-B02	3
Fagron	Ácido salicílico	14L02B02303557	1
Fagron	Ácido salicílico	14L02-B02-303557	12
Fagron	Ácido salicílico	14L02B02303558	1
Fagron	Ácido salicílico	14L02-B02-303558	16
Fagron	Ácido salicílico	15211806	2
Fagron	Ácido salicílico	15211809	1
Fagron	Ácido salicílico	16/15-B08-330773	3
Fagron	Ácido salicílico	16/15-B08-331442	1
Fagron	Ácido salicílico	16/15-B08-332098	2
Fagron	Ácido salicílico	16/15-B08-333933	3
Fagron	Ácido salicílico	1615-B08-330773	1
Fagron	Ácido salicílico	1615B08332098	1
Fagron	Ácido salicílico	16A18-B04	2
Fagron	Ácido salicílico	16A18-B04322904	1
Fagron	Ácido salicílico	16A18-B04-322904	3
Fagron	Ácido salicílico	16A18-B04-322905	2
Fagron	Ácido salicílico	16A18B04322905	2
Fagron	Ácido salicílico	16E02-B09-325355	1
Fagron	Ácido salicílico	16E02-B09-325356	2
Fagron	Ácido salicílico	16I15-B08	1
Fagron	Ácido salicílico	16I15-B08-327353	2
Fagron	Ácido salicílico	16I15B08330773	1
Fagron	Ácido salicílico	16I15-B08-330773	1
Fagron	Ácido salicílico	16I15-B08-332098	1
Fagron	Ácido salicílico	16I15-B08-333932	3
Fagron	Ácido salicílico	17301502	1
Fagron	Ácido salicílico	17C21B09	1
Fagron	Ácido salicílico	17C21-B09	2
Fagron	Ácido salicílico	17c21-b09-337172	1
Fagron	Ácido salicílico	17C21-B09-337172	3
Fagron	Ácido salicílico	17C21-B09-337173	4
Fagron	Ácido salicílico	17c21-b09-337860	1
Fagron	Ácido salicílico	17C21-B09-337860	3
Fagron	Ácido salicílico	1801042-01	1
Fagron	Ácido salicílico	18E24-B03	1
Fagron	Ácido salicílico	18E24-B03-354310	3
Fagron	Ácido salicílico	18E24-B03-354311	3
Fagron	Ácido salicílico	18E24-B03-354312	1
Fagron	Ácido salicílico	18F05-B02	2
Fagron	Ácido salicílico	18F05-B02-350586	6
Fagron	Ácido salicílico	18F05B02350587	2
Fagron	Ácido salicílico	18F05-B02-350587	8
Fagron	Ácido salicílico	18F05-B02-351974	3
Fagron	Ácido salicílico	18F05-B02-352210	2
Fagron	Ácido salicílico	18F05-B02-352528	1
Fagron	Ácido salicílico	18F15-B02-350587	1
Fagron	Ácido salicílico	1901015-03	1
Fagron	Ácido salicílico	190262	1
Fagron	Ácido salicílico	190263	20
Fagron	Ácido salicílico	190263RAS1818100	1
Fagron	Ácido salicílico	190264	15
Fagron	Ácido salicílico	19B12-B04	2
Fagron	Ácido salicílico	19B12-B04-193458	1
Fagron	Ácido salicílico	19B12-B04-193459	2
Fagron	Ácido salicílico	19B12-B04-193460	7
Fagron	Ácido salicílico	20A29-B31	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ácido salicílico	20A29-B31-197697	6
Fagron	Ácido salicílico	20E21-B03	5
Fagron	Ácido salicílico	20e21-B03-200496	1
Fagron	Ácido salicílico	20E21B03200496	1
Fagron	Ácido salicílico	20E21-B03-200496	8
Fagron	Ácido salicílico	20E21-Bo3-200496	1
Fagron	Ácido salicílico	20E21-BO3-200496	1
Fagron	Ácido salicílico	20E32-B03-200496	1
Fagron	Ácido salicílico	20G20-B04	1
Fagron	Ácido salicílico	20G20-B04-202192	3
Fagron	Ácido salicílico	20G20-B04-202193	1
Fagron	Ácido salicílico	21003008004	1
Fagron	Ácido salicílico	21A26-B19-210110	3
Fagron	Ácido salicílico	21a26-b19-210141	1
Fagron	Ácido salicílico	21A26-B19-210141	3
Fagron	Ácido salicílico	21G21-BO4-217748	1
Fagron	Ácido salicílico	21G30B03215511	1
Fagron	Ácido salicílico	21G30-B03-215511	6
Fagron	Ácido salicílico	21G3O-BO3-2155101	1
Fagron	Ácido salicílico	21J06B11-217750	1
Fagron	Ácido salicílico	21J06-B11-217750	2
Fagron	Ácido salicílico	2201115	1
Fagron	Ácido salicílico	22E12-B05-224210	1
Fagron	Ácido salicílico	290852	1
Fagron	Ácido salicílico	3111Q-01045	1
Fagron	Ácido salicílico	AS28012021	1
Fagron	Ácido salicílico	B03-2004906	2
Fagron	Ácido salicílico	B19-210110	1
Fagron	Ácido salicílico	B31-1976907	3
Fagron	Ácido salicílico	RAS1135100	1
Fagron	Ácido salicílico	RAS1135300	1
Fagron	Ácido salicílico	RAS1808500	1
Fagron	Ácido salicílico	RAS1818100	4
Fagron	Ácido salicílico	RAS1929500	1
Fagron	Ácido salicílico	xxxxxxxx	1
Fargon / AHD	Ácido salicílico	20E21-B03-200496	2
Fargon	Ácido salicílico	14L02-B02	1
Farmalabor / Farmalabor	Ácido salicílico	P1404195-002	1
Fiebig/Maros	Ácido salicílico	1707009-02	1
Fiebig	Ácido salicílico	15211810	1
Fiebig	Ácido salicílico	16010905	1
Fiebig	Ácido salicílico	17301506	1
Fiebig	Ácido salicílico	17301509	1
Fiebig	Ácido salicílico	18147321	1
Gatt-Koller	Ácido salicílico	1803840	2
Gehe / Spinnrad	Ácido salicílico	16050005	1
Gehe amax	Ácido salicílico	12036223	1
Gehe amax	Ácido salicílico	1801042-01	1
Gehe amax	Ácido salicílico	18147302	1
Gehe amax	Ácido salicílico	18147314	1
Gehe/ Caesar & Loret…	Ácido salicílico	20000146005	1
Gehe	Ácido salicílico		1
Gehe	Ácido salicílico	1050313	1
Gehe	Ácido salicílico	11D15-N08	1
Gehe	Ácido salicílico	1206007-01	1
Gehe	Ácido salicílico	13B14-N01	1
Gehe	Ácido salicílico	13H01-N04	1
Gehe	Ácido salicílico	14336919	1
Gehe	Ácido salicílico	14E26-B04-294624	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Ácido salicílico	14L02-B02-303558	1
Gehe	Ácido salicílico	15217301	1
Gehe	Ácido salicílico	15217304	1
Gehe	Ácido salicílico	16010910	1
Gehe	Ácido salicílico	16050013	1
GEHE	Ácido salicílico	1605023-01	1
GEHE	Ácido salicílico	1605023-02	2
Gehe	Ácido salicílico	16312003	1
Gehe	Ácido salicílico	165023-02	1
gehe	Ácido salicílico	16I15-B08-331442	1
Gehe	Ácido salicílico	1707009-01	1
GEHE	Ácido salicílico	1707009-01	1
GEHE	Ácido salicílico	1707009-02	1
Gehe	Ácido salicílico	17133301	1
Gehe	Ácido salicílico	17133307	4
GEHE	Ácido salicílico	17301502	2
Gehe	Ácido salicílico	17301511	1
GEHE	Ácido salicílico	17301511	1
Gehe	Ácido salicílico	17C21-B09-337172	1
Gehe	Ácido salicílico	18147308	2
Gehe	Ácido salicílico	18147314	1
GEHE	Ácido salicílico	18147317	1
Gehe	Ácido salicílico	18147321	1
Gehe	Ácido salicílico	18230007	1
GEHE	Ácido salicílico	18230009	1
Gehe	Ácido salicílico	18F05-B02-350586	1
Gehe	Ácido salicílico	20000147002	1
Gehe	Ácido salicílico	20000147004	1
Gehe	Ácido salicílico	20000147006	2
Gehe	Ácido salicílico	20003823008	2
Gehe	Ácido salicílico	2000442010	2
Gehe	Ácido salicílico	20004424015	1
Gehe	Ácido salicílico	21003008010	1
Gehe	Ácido salicílico	21003008016	1
GEHE	Ácido salicílico	22001529002	1
gehe	Ácido salicílico	22003107004	1
Gehe	Ácido salicílico	2208003-01	1
Gehe	Ácido salicílico	2208003-02	1
Gehe	Ácido salicílico	22D07-B03-221811	2
gehe	Ácido salicílico	2308012-01	1
Gehe	Ácido salicílico	2308012-01	1
Gehe	Ácido salicílico	24000043001	1
Geibo 5.7.21	Ácido salicílico	20A29-B31-197697	1
Geilenkirchen	Ácido salicílico	17301506	1
Geilenkirchen	Ácido salicílico	192209001	2
Gutenberg-Apotheke	Ácido salicílico	12374208	1
Hänseler	Ácido salicílico		7
Hofmann & Sommer	Ácido salicílico	1230	3
Holdermann	Ácido salicílico	14E26-B04294624	1
Ichthyol/ Noweda	Ácido salicílico	17133303	1
Ichthyol/Noweda	Ácido salicílico	13344003	1
Ichthyol	Ácido salicílico	11311922	2
Jenne	Ácido salicílico	12345	1
Jenne	Ácido salicílico	18147314	1
Jenne	Ácido salicílico	20000147004	1
Jenne	Ácido salicílico	20003823016	2
Jenne	Ácido salicílico	22J26B06-227888	1
Kehr	Ácido salicílico	16312001	2
Kehr	Ácido salicílico	16312012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Ácido salicílico	17301509	1
Kehr	Ácido salicílico	2201044-02	1
Kehr	Ácido salicílico	23003599002	1
Klenk	Ácido salicílico	12134722	1
Krieger	Ácido salicílico	13032017-MW-A	1
Krieger	Ácido salicílico	16050012	1
L30	Ácido salicílico	16312005	1
L30	Ácido salicílico	17301505	1
L30	Ácido salicílico	17301507	1
Midas	Ácido salicílico	16312010	1
Novacyl / Ebert	Ácido salicílico	14336911	2
Novacyl / Ebert	Ácido salicílico	14336919	1
Novacyl / Gehe	Ácido salicílico	16010912	1
Novacyl / Gehe	Ácido salicílico	18147321	1
Novacyl, FR	Ácido salicílico	15084403	2
Novacyl/Caesar & Lor…	Ácido salicílico	17301505	1
Novacyl/Gehe Pharma …	Ácido salicílico	17301507	1
Novacyl/Phoenix	Ácido salicílico	RAS1817400	1
Novacyl/Phoenix	Ácido salicílico	RAS1818100	2
Novacyl/Phoenix	Ácido salicílico	RAS1907500	1
Novacyl	Ácido salicílico	1707009-02	1
Novacyl	Ácido salicílico	1910018-01	1
Novacyl	Ácido salicílico	RAS1821600	1
Noweda/ Caesar&Loren…	Ácido salicílico	192209001	1
Noweda/ Infecto Pharm	Ácido salicílico	16/15-08-330773	1
Noweda/Fargon	Ácido salicílico	14L02-B02-303556	1
Noweda	Ácido salicílico	12036215	1
Noweda	Ácido salicílico	12036226	1
Noweda	Ácido salicílico	1406027-01	1
Noweda	Ácido salicílico	140602702	1
Noweda	Ácido salicílico	14336907	2
Noweda	Ácido salicílico	16/15-B08-330773	1
Noweda	Ácido salicílico	16050011	1
Noweda	Ácido salicílico	16050013	1
Noweda	Ácido salicílico	1707009-02	2
Noweda	Ácido salicílico	170700904	3
Noweda	Ácido salicílico	17133304	1
noweda	Ácido salicílico	17301502	1
Noweda	Ácido salicílico	17304506	1
Noweda	Ácido salicílico	180104201	1
Noweda	Ácido salicílico	181473001	2
Noweda	Ácido salicílico	1901015	1
Noweda	Ácido salicílico	1901015-01	1
Noweda	Ácido salicílico	1901015-03	1
Noweda	Ácido salicílico	190263	1
Noweda	Ácido salicílico	19061206	1
Noweda	Ácido salicílico	19B12-B04-193459	1
Noweda	Ácido salicílico	20003823008	1
noweda	Ácido salicílico	20004424015	1
Noweda	Ácido salicílico	210802401	1
Noweda	Ácido salicílico	22001524003	1
Noweda	Ácido salicílico	22001528002	1
Noweda	Ácido salicílico	22001528003	2
Noweda	Ácido salicílico	22001529002	1
noweda	Ácido salicílico	22001534003	1
Noweda	Ácido salicílico	2208003_01	1
Noweda	Ácido salicílico	2208003-02	1
Noweda	Ácido salicílico	AS10052021	1
Noweda	Ácido salicílico	P2021/113	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix 09.10.2017	Ácido salicílico	16050017	1
Phoenix goettingen	Ácido salicílico	14300808	1
Phoenix/Cealo	Ácido salicílico	1733303	1
Phoenix/Cealo	Ácido salicílico	3414M-01045	1
Phoenix	Ácido salicílico	12H10-No8	1
Phoenix	Ácido salicílico	14076201	1
Phoenix	Ácido salicílico	15211808	2
Phoenix	Ácido salicílico	16050012	1
Phoenix	Ácido salicílico	16312005	1
Phoenix	Ácido salicílico	17301502	1
Phoenix	Ácido salicílico	18050007	1
Phoenix	Ácido salicílico	18147308	1
Phoenix	Ácido salicílico	19061202	1
Phoenix	Ácido salicílico	1910018-02	1
Phoenix	Ácido salicílico	191411012	1
Phoenix	Ácido salicílico	20004424006	1
Phoenix	Ácido salicílico	20004424007	1
Phoenix	Ácido salicílico	22001529002	1
Phoenix	Ácido salicílico	22001534003	2
Phoenix	Ácido salicílico	2208003-01	1
Phoenox	Ácido salicílico	20000147004	1
Phönix 02.08.2019	Ácido salicílico	18230009	1
Phönix Gotha	Ácido salicílico	12374207	1
Phönix Gotha	Ácido salicílico	14076201	1
Phönix Gotha	Ácido salicílico	14300801	1
Phönix Gotha	Ácido salicílico	18050006	1
Phönix	Ácido salicílico	11311917	1
Phönix	Ácido salicílico	12323401	1
Phönix	Ácido salicílico	12374210	1
Phönix	Ácido salicílico	12374211	1
Phönix	Ácido salicílico	12C20-N12	1
Phönix	Ácido salicílico	1303020-01	3
Phönix	Ácido salicílico	13K08-B31-290853	1
Phönix	Ácido salicílico	1509007-02	1
Phönix	Ácido salicílico	16050005	1
Phönix	Ácido salicílico	16050012	1
Phönix	Ácido salicílico	16a18-b04-322905	1
Phönix	Ácido salicílico	1713303	1
Phönix	Ácido salicílico	17301506	1
Phönix	Ácido salicílico	17301507	1
Phonix	Ácido salicílico	18050007	1
Phönix	Ácido salicílico	18050009	5
Phönix	Ácido salicílico	18147302	1
Phönix	Ácido salicílico	18147303	2
Phönix	Ácido salicílico	18147314	2
Phönix	Ácido salicílico	190612001	1
Phönix	Ácido salicílico	200004424001	1
phönix	Ácido salicílico	20004424004	1
Phönix	Ácido salicílico	20004424004	1
Phönix	Ácido salicílico	20004424006	1
Phönix	Ácido salicílico	2101028-01	1
Phönix	Ácido salicílico	2108024-01	2
Phönix	Ácido salicílico	22001529002	2
Phönix	Ácido salicílico	22001534003	1
Phönix	Ácido salicílico	3177	1
Phönix	Ácido salicílico	68/AKD4	1
Röntgen	Ácido salicílico	190612004	1
Salicylsäure	Ácido salicílico	190612001	1
Sana 04.02.17 Ek:13,83	Ácido salicílico	16010910	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp 28.01.15 EK…	Ácido salicílico	14076204	1
Sanacorp	Ácido salicílico	11311922	1
Sanacorp	Ácido salicílico	12134707	1
Sanacorp	Ácido salicílico	12134712	1
Sanacorp	Ácido salicílico	12134715	1
Sanacorp	Ácido salicílico	123036223	1
Sanacorp	Ácido salicílico	12374205	1
Sanacorp	Ácido salicílico	12374210	1
Sanacorp	Ácido salicílico	1303020-01	1
Sanacorp	Ácido salicílico	13344014	1
Sanacorp	Ácido salicílico	13344018	1
Sanacorp	Ácido salicílico	15084404	1
Sanacorp	Ácido salicílico	16010910	1
Sanacorp	Ácido salicílico	16010912	1
Sanacorp	Ácido salicílico	16050005	1
Sanacorp	Ácido salicílico	16050012	1
Sanacorp	Ácido salicílico	17133307	1
Sanacorp	Ácido salicílico	171333307	1
Sanacorp	Ácido salicílico	17301505	1
Sanacorp	Ácido salicílico	17301506	1
Sanacorp	Ácido salicílico	17301509	1
Sanacorp	Ácido salicílico	17C21-B09-339446	1
Sanacorp	Ácido salicílico	18050006	1
Sanacorp	Ácido salicílico	18050007	1
Sanacorp	Ácido salicílico	18147303	1
Sanacorp	Ácido salicílico	1910018-03	1
Sanacorp	Ácido salicílico	20000147002	1
Sanacorp	Ácido salicílico	2000442406	1
Sanacorp	Ácido salicílico	20E21-B03-200496	1
Sanacorp	Ácido salicílico	2101028-01	1
Sanacorp	Ácido salicílico	21A26-B19-210110	1
sanacorp	Ácido salicílico	22001528002	1
Sanacorp	Ácido salicílico	22001529002	1
Sanacorp	Ácido salicílico	22001534003	1
Sanacorp	Ácido salicílico	23002014003	1
Sanacorp	Ácido salicílico	68/AKD2	1
Spangropharm	Ácido salicílico	11197104	1
VDL	Ácido salicílico	11197122	1
VDL	Ácido salicílico	22D07-B03-221811	1
xxx	Ácido salicílico	4311A-01045	1

- 231 760 spectra from 1515 *Apo-Ident* customers from a total of 48 672 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido salicílico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido salicílico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	1120	0	200 964
Type C	0	4283	24	231 760

The substance/substance group *Ácido salicílico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4643 %)
Type C	100.0000 % (> 99.9007 %)	99.4428 % (> 99.3731 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20696	21906	6,53	218,15
21436	21906	6,44	218,53
21760	21906	2,74	221,03
21906	21906	0,00	221,18
22443	22443	0,00	210,55
23592	21906	3,47	222,12
24591	21906	4,97	222,14
25543	25543	0,00	220,90
26113	26113	0,00	213,34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido sórbico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20881-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido sórbico; Acidum sorbicum

Special notes

When selecting the *Ácido sórbico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido sórbico	9	3	110

Second-stage model

For differentiation of the substance/substance group *Ácido sórbico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido sórbico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	81,33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido sórbico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido sórbico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido sórbico	12038025	20881	40	20120315
Caelo	Ácido sórbico	13334008	21460	60	AR-15-FG-007849-01
Caelo	Ácido sórbico	14380714	22593	40	20150209
Caelo	Ácido sórbico	162080	22616	40	20160722*
Caelo	Ácido sórbico	15382002	22826	40	20151112
Caelo	Ácido sórbico	172056	23851	40	20170823*
Caelo	Ácido sórbico	162080	23859	40	20160722*
Caelo	Ácido sórbico	20002774	25615	40	20200910*
Caelo	Ácido sórbico	22000825	26120	40	20220513*
Caelo	Ácido sórbico	22000825	26120SI	20	20220513*
Caelo	Ácido sórbico	23002243	26951	40	20230914*
Caelo	Ácido sórbico	23002243	26951SI	20	20230914*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 12 reference samples from the substance/substance group *Ácido sórbico*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 502 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Ácido sórbico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido sórbico	14176214	22592	40
Caelo	Ácido sórbico	182876	24384	40
Caelo	Ácido sórbico	191114	24569	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 772 spectra from 459 *Apo-Ident* customers from 117 batches from the substance/substance group *Ácido sórbico*.

- Among them are spectra of independent samples from 110 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido sórbico	22000825005	1
	Ácido sórbico	22000825006	1
	Ácido sórbico	22000825009	1
	Ácido sórbico	22000825011	1
	Ácido sórbico	22000825015	1
	Ácido sórbico	22000825016	3
	Ácido sórbico	22000825020	4
	Ácido sórbico	22000825105	1
	Ácido sórbico	22000825106	1
	Ácido sórbico	23002243003	2
acidum sorbicum	Ácido sórbico	17343411	1
AHD	Ácido sórbico	22000825020	1
ALH	Ácido sórbico	15382007	1
Alliance Healthcare	Ácido sórbico	20000110010	1
Alliance Healthcare	Ácido sórbico	20004209014	1
Alliance	Ácido sórbico	22000825020	1
Anzag	Ácido sórbico	12038016	1
Caelo	Ácido sórbico		1
Caelo	Ácido sórbico	10120303	1
Caelo	Ácido sórbico	10305208	1
Caelo	Ácido sórbico	10305209	1
Caelo	Ácido sórbico	105505	1
Caelo	Ácido sórbico	11203806	2
Caelo	Ácido sórbico	11203807	10
Caelo	Ácido sórbico	11203812	1
Caelo	Ácido sórbico	12038002	1
Caelo	Ácido sórbico	12038009	1
Caelo	Ácido sórbico	12038012	1
Caelo	Ácido sórbico	12038016	6
Caelo	Ácido sórbico	12038020	4
Caelo	Ácido sórbico	12038025	1
Caelo	Ácido sórbico	12330608	8
Caelo	Ácido sórbico	12330618	12
Caelo	Ácido sórbico	13334003	4
Caelo	Ácido sórbico	13334008	6
Caelo	Ácido sórbico	13334010	7
Caelo	Ácido sórbico	14176206	7
Caelo	Ácido sórbico	14176207	1
Caelo	Ácido sórbico	14176209	6
Caelo	Ácido sórbico	14176212	8
Caelo	Ácido sórbico	14176213	1
Caelo	Ácido sórbico	14176214	12
Caelo	Ácido sórbico	14380702	3
Caelo	Ácido sórbico	14380704	1
Caelo	Ácido sórbico	14380706	6
Caelo	Ácido sórbico	14380713	2
Caelo	Ácido sórbico	14380714	11
Caelo	Ácido sórbico	14380715	1
Caelo	Ácido sórbico	15123912	1
Caelo	Ácido sórbico	15382001	1
Caelo	Ácido sórbico	15382002	12
Caelo	Ácido sórbico	15382007	4
Caelo	Ácido sórbico	15382010	15
Caelo	Ácido sórbico	16206012	1
Caelo	Ácido sórbico	162080	1
Caelo	Ácido sórbico	16208005	30
Caelo	Ácido sórbico	16208007	1
Caelo	Ácido sórbico	16208009	22
Caelo	Ácido sórbico	16208011	13
Caelo	Ácido sórbico	16208012	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido sórbico	16208015	12
Caelo	Ácido sórbico	16208016	18
Caelo	Ácido sórbico	16208018	2
Caelo	Ácido sórbico	16208020	18
Caelo	Ácido sórbico	1620808005	1
Caelo	Ácido sórbico	162508016	1
Caelo	Ácido sórbico	170427AS/16208005	1
Caelo	Ácido sórbico	1734301	1
Caelo	Ácido sórbico	17343401	17
Caelo	Ácido sórbico	17343411	26
Caelo	Ácido sórbico	17343411P-190225-13	1
Caelo	Ácido sórbico	17343422	16
Caelo	Ácido sórbico	18215610	1
Caelo	Ácido sórbico	1827669	1
Caelo	Ácido sórbico	18284605	1
Caelo	Ácido sórbico	18286716	1
Caelo	Ácido sórbico	18287602	2
Caelo	Ácido sórbico	18287605	30
Caelo	Ácido sórbico	18287609	27
Caelo	Ácido sórbico	18287616	22
Caelo	Ácido sórbico	18287616P-191111-5	1
Caelo	Ácido sórbico	1887618	1
Caelo	Ácido sórbico	191114	1
Caelo	Ácido sórbico	191114001	20
Caelo	Ácido sórbico	191114002	22
Caelo	Ácido sórbico	19111405	1
Caelo	Ácido sórbico	19114002	2
Caelo	Ácido sórbico	200000110010	1
Caelo	Ácido sórbico	20000110010	6
Caelo	Ácido sórbico	200004209003	2
Caelo	Ácido sórbico	20004209003	24
Caelo	Ácido sórbico	20004209011	15
Caelo	Ácido sórbico	20004209014	17
Caelo	Ácido sórbico	2000420911	1
Caelo	Ácido sórbico	200042209011	1
Caelo	Ácido sórbico	21041801	1
Caelo	Ácido sórbico	22000825005	4
Caelo	Ácido sórbico	22000825006	4
Caelo	Ácido sórbico	22000825009	2
Caelo	Ácido sórbico	22000825015	1
Caelo	Ácido sórbico	22000825016	5
Caelo	Ácido sórbico	22000825020	1
Caelo	Ácido sórbico	28041726	1
Caelo	Ácido sórbico	29071201	1
Caelo	Ácido sórbico	4016I-01048	1
Caelo	Ácido sórbico	4811Q-01048	1
Caelo	Ácido sórbico	5012E-01048	1
Caelo	Ácido sórbico	72687038	1
Caelo	Ácido sórbico	80538258	1
Caelo	Ácido sórbico	9280207	1
Caelo	Ácido sórbico	93557220	2
Caelo	Ácido sórbico	P0538258	1
Caeo/ Phoenix	Ácido sórbico	18287616	1
Caesar & Lorenz GmbH	Ácido sórbico	18287609	1
Caesar & Loretz GmbH...	Ácido sórbico	191114001	1
Caesar & Loretz GmbH...	Ácido sórbico	18287616	1
Caesar & Loretz GmbH...	Ácido sórbico	16208009	1
Caesar & Loretz GmbH...	Ácido sórbico	191114002	1
Caesar & Loretz GmbH...	Ácido sórbico	18287616	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Ácido sórbico	19111405	1
Caesar & Loretz GmbH...	Ácido sórbico	22000825006	1
Caesar & Loretz GmbH...	Ácido sórbico	20000110005	1
Caesar & Loretz GmbH...	Ácido sórbico	19111406	1
Caesar & Loretz GmbH/Gehe	Ácido sórbico	191114001	1
Caesar & Loretz GmbH/Gehe	Ácido sórbico	191114002	1
Caesar & Loretz GmbH/Gehe	Ácido sórbico	22000825006	2
Caesar & Loretz GmbH...	Ácido sórbico	18287609	1
Caesar & Loretz GmbH...	Ácido sórbico	191114001	1
Caesar & Loretz GmbH...	Ácido sórbico	20004209003	1
Caesar & Loretz GmbH/K	Ácido sórbico	20004209014	1
Caesar & Loretz GmbH...	Ácido sórbico	191114001	1
Caesar & Loretz GmbH...	Ácido sórbico	20000110005	1
Caesar & Loretz GmbH...	Ácido sórbico	20000110010	1
Caesar & Loretz GmbH...	Ácido sórbico	20004209003	1
Caesar & Loretz GmbH/Sana	Ácido sórbico	18287606	1
Caesar & Loretz GmbH...	Ácido sórbico	191114005	1
Caesar & Loretz GmbH...	Ácido sórbico	20000110010	1
Caesar & Loretz GmbH...	Ácido sórbico	20004209003	1
Caesar & Loretz GmbH...	Ácido sórbico	20004209006	1
Caesar & Loretz GmbH...	Ácido sórbico	20004209011	1
Caesar & Loretz GmbH...	Ácido sórbico	22000825016	1
Caesar & Loretz GmbH	Ácido sórbico	18287605	7
Caesar & Loretz GmbH	Ácido sórbico	18287609	7
Caesar & Loretz GmbH	Ácido sórbico	18287615	1
Caesar & Loretz GmbH	Ácido sórbico	18287616	12
Caesar & Loretz GmbH	Ácido sórbico	191114001	11
Caesar & Loretz GmbH	Ácido sórbico	191114002	2
Caesar & Loretz GmbH	Ácido sórbico	20000110010	2
Caesar & Loretz GmbH	Ácido sórbico	20004209002	1
Caesar & Loretz GmbH	Ácido sórbico	20004209003	7
Caesar & Loretz GmbH	Ácido sórbico	20004209008	1
Caesar & Loretz GmbH	Ácido sórbico	20004209010	4
Caesar & Loretz GmbH	Ácido sórbico	20004209011	2
Caesar & Loretz GmbH	Ácido sórbico	20004209014	9
Caesar & Loretz GmbH	Ácido sórbico	22000825006	1
Caesar & Loretz GmbH	Ácido sórbico	22000825009	1
Caesar & Loretz GmbH	Ácido sórbico	22000825020	1
Caesar & Loretz GmbH	Ácido sórbico	22000825105	1
Caesar & Loretz GmbH	Ácido sórbico	22000825106	1
Caesar & Loretz/Noweda	Ácido sórbico	14380706	1
Caesar/Gehe	Ácido sórbico	17343422	1
Cealo/Gehe	Ácido sórbico	22000825009	1
Cealo	Ácido sórbico	16208011	1
Ebert & Jacobi	Ácido sórbico	16208005	1
Euro OTC	Ácido sórbico	12038020	1
Euro OTC	Ácido sórbico	o216E-01048	1
Fagron	Ácido sórbico	121394	1
Fagron	Ácido sórbico	13334008	1
Fagron	Ácido sórbico	14176206	1
Fagron	Ácido sórbico	17343422	1
Fiebig	Ácido sórbico	168009	1
Finze	Ácido sórbico	9280207	1
Fischar	Ácido sórbico	16208005	1
Gatt-Koller / Phoenix	Ácido sórbico	2575/07142914	1
Gehe Rostock	Ácido sórbico	191114001	1
Gehe	Ácido sórbico	16208011	1
Gehe	Ácido sórbico	16208012	1
gehe	Ácido sórbico	16208016	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Ácido sórbico	17343401	1
GEHE	Ácido sórbico	17343401	1
Gehe	Ácido sórbico	18287605	1
Gehe	Ácido sórbico	18287609	2
Gehe	Ácido sórbico	191114002	1
Gehe	Ácido sórbico	20004209011	1
Geilenkirchen	Ácido sórbico	16208009	1
H.Lamotte	Ácido sórbico	17343401	1
L12	Ácido sórbico	15382010	1
L12	Ácido sórbico	18287602	1
Noweda	Ácido sórbico	12038016	1
Noweda	Ácido sórbico	12330608	1
Noweda	Ácido sórbico	14176206	1
Noweda	Ácido sórbico	1418M-01048	1
Noweda	Ácido sórbico	14380706	1
Noweda	Ácido sórbico	16208020	1
Noweda	Ácido sórbico	18287605	3
Noweda	Ácido sórbico	18287609	1
Noweda	Ácido sórbico	20000110010	1
Noweda	Ácido sórbico	22000825011	1
Noweda	Ácido sórbico	22000825020	1
Phoenix 17.4.13	Ácido sórbico	12038020	1
PHOENIX 12.05.2014	Ácido sórbico	13334008	1
Phoenix 22.03.2017 6,67EUR	Ácido sórbico	15382010	1
Phoenix	Ácido sórbico	11203813	1
Phoenix	Ácido sórbico	191114001	1
Phoenix	Ácido sórbico	20004209003	1
Phönix	Ácido sórbico	12330618	1
phönix	Ácido sórbico	15382010	1
Phönix	Ácido sórbico	16208005	1
Phönix	Ácido sórbico	16208020	1
Phönix	Ácido sórbico	18287605	1
Phönix	Ácido sórbico	20000110010	1
PHÖNIX	Ácido sórbico	9308627	1
Sanacorp	Ácido sórbico	12038016	1
Sanacorp	Ácido sórbico	13334008	1
Sanacorp	Ácido sórbico	16208020	1
Sanacorp	Ácido sórbico	18287605	2
Sanacorp	Ácido sórbico	20004209003	1
Sanacorp	Ácido sórbico	22000825006	1
Sanacorp	Ácido sórbico	22000825008	1
SanacorpWE: 23.09.14...	Ácido sórbico	14176212	1
Th. Geyer	Ácido sórbico	17343411	1
vdl 28.04.2014 preis:5,79	Ácido sórbico		1
VDL;5,78EUR;18.12	Ácido sórbico	14176206	1

- 235 295 spectra from 1515 *Apo-Ident* customers from a total of 49 143 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido sórbico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido sórbico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	120	0	201 964
Type C	0	772	0	235 295

The substance/substance group *Ácido sórbico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.2228 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20881	23859	7,07	140,34
21460	21460	0,00	140,45
22593	23859	5,59	141,38
22616	22616	0,00	145,13
22826	21460	8,19	137,43
23851	23851	0,00	139,52
23859	23859	0,00	139,82
25615	25615	0,00	137,01
26120	26120	0,00	151,97
26951	26951	0,00	159,36

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido tartárico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20014-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido tartárico; Acidum tartaricum

Special notes

When selecting the *Ácido tartárico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido tartárico	10	4	172

Second-stage model

For differentiation of the substance/substance group *Ácido tartárico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido tartárico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	87,05	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido tartárico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido tartárico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ácido tartárico	15130201	22383	60	20150416
Caelo	Ácido tartárico	15164001	22384	60	1704461
Caelo	Ácido tartárico	161468	22613	40	20160607*
Caelo	Ácido tartárico	21000301	25628	40	20210301*
Caelo	Ácido tartárico	21000938	25699	50	20210430*
Caelo	Ácido tartárico	24001998	27307	40	20240906*
Caelo	Ácido tartárico	24001998	27307SI	20	20240906*
Euro OTC	Ácido tartárico	1907022	24806	40	20190813*
Fagron	Ácido tartárico	13I25-B01-294093	22391	60	1711509
Fagron	Ácido tartárico	14G07-B02-308554	22501	40	20140827
Fagron	Ácido tartárico	21J15-B03-220487	26397	40	20220126
Fagron	Ácido tartárico	21J15-B03-220487	26397SI	20	20220126

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 510 spectra of 12 reference samples from the substance/substance group *Ácido tartárico*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 452 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 4 reference samples from the substance/substance group *Ácido tartárico*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ácido tartárico	13217803	21457	60
Caelo	Ácido tartárico	181212	24015	40
Caelo	Ácido tartárico	21002221	25799	50
Fagron	Ácido tartárico	14G07-B02-322976	23527	40

- 201 894 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 440 spectra from 210 *Apo-Ident* customers from 180 batches from the substance/substance group *Ácido tartárico*.

- Among them are spectra of independent samples from 171 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido tartárico	20J05B01202754	1
	Ácido tartárico	21000301006	1
	Ácido tartárico	23000312004	1
apomix	Ácido tartárico		1
apomix	Ácido tartárico	1111	1
Beiersdorf AG	Ácido tartárico	11G19-N08	2
Caelo	Ácido tartárico		1
Caelo	Ácido tartárico	10073105	1
Caelo	Ácido tartárico	10180708	2
Caelo	Ácido tartárico	10180713	2
Caelo	Ácido tartárico	10180714	1
Caelo	Ácido tartárico	10199713	1
Caelo	Ácido tartárico	11169406	2
Caelo	Ácido tartárico	1169406	1
Caelo	Ácido tartárico	11k10-n07	1
Caelo	Ácido tartárico	1204102	1
Caelo	Ácido tartárico	12044101	2
Caelo	Ácido tartárico	12044102	3
Caelo	Ácido tartárico	12044103	4
Caelo	Ácido tartárico	12044119	3
Caelo	Ácido tartárico	12240402	1
Caelo	Ácido tartárico	12240413	1
Caelo	Ácido tartárico	12240415	1
Caelo	Ácido tartárico	12286903	2
Caelo	Ácido tartárico	12286904	2
Caelo	Ácido tartárico	12286906	4
Caelo	Ácido tartárico	12286911	1
Caelo	Ácido tartárico	12286924	1
Caelo	Ácido tartárico	12286932	1
Caelo	Ácido tartárico	12286934	1
Caelo	Ácido tartárico	12286939	1
Caelo	Ácido tartárico	12H02-n07	1
Caelo	Ácido tartárico	13116306	1
Caelo	Ácido tartárico	13116307	1
Caelo	Ácido tartárico	13116308	2
Caelo	Ácido tartárico	13217803	1
Caelo	Ácido tartárico	13217806	2
Caelo	Ácido tartárico	13217807	1
Caelo	Ácido tartárico	13B15-N01	2
Caelo	Ácido tartárico	13125-B01-294093	1
Caelo	Ácido tartárico	14054521	1
Caelo	Ácido tartárico	14186211	1
Caelo	Ácido tartárico	14186213	4
Caelo	Ácido tartárico	14G07-B02-308555	2
Caelo	Ácido tartárico	14G07-B02-330640	1
Caelo	Ácido tartárico	15045303	1
Caelo	Ácido tartárico	15045304	1
Caelo	Ácido tartárico	151302	1
Caelo	Ácido tartárico	15130201	6
Caelo	Ácido tartárico	15130205	2
Caelo	Ácido tartárico	15130206	1
Caelo	Ácido tartárico	15130207	1
Caelo	Ácido tartárico	15164001	4
Caelo	Ácido tartárico	15164002	3
Caelo	Ácido tartárico	15164008	5
Caelo	Ácido tartárico	15164010	1
Caelo	Ácido tartárico	15349101	5
Caelo	Ácido tartárico	15349102	5
Caelo	Ácido tartárico	15349105	9
Caelo	Ácido tartárico	15349106	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ácido tartárico	15349109	5
Caelo	Ácido tartárico	15349110	2
Caelo	Ácido tartárico	16146806	2
Caelo	Ácido tartárico	16146809	1
Caelo	Ácido tartárico	16146811	1
Caelo	Ácido tartárico	16260403	5
Caelo	Ácido tartárico	16260404	5
Caelo	Ácido tartárico	16260405	1
Caelo	Ácido tartárico	16260406	5
Caelo	Ácido tartárico	17091402	1
Caelo	Ácido tartárico	17337504	2
Caelo	Ácido tartárico	17337505	3
Caelo	Ácido tartárico	17337506	2
Caelo	Ácido tartárico	17347103	5
Caelo	Ácido tartárico	17347104	3
Caelo	Ácido tartárico	1812104	1
Caelo	Ácido tartárico	18121201	1
Caelo	Ácido tartárico	18121204	6
Caelo	Ácido tartárico	18121205	1
Caelo	Ácido tartárico	18121208	6
Caelo	Ácido tartárico	18121210	5
Caelo	Ácido tartárico	18121211	9
Caelo	Ácido tartárico	18121212	3
Caelo	Ácido tartárico	18121214	9
Caelo	Ácido tartárico	182394004	1
Caelo	Ácido tartárico	18239403	1
Caelo	Ácido tartárico	18239405	1
Caelo	Ácido tartárico	18239406	3
Caelo	Ácido tartárico	18239407	3
Caelo	Ácido tartárico	18239407/P-04121921	1
Caelo	Ácido tartárico	191825002	10
Caelo	Ácido tartárico	191825003	13
Caelo	Ácido tartárico	191825004	2
Caelo	Ácido tartárico	191825006	2
Caelo	Ácido tartárico	19182502	1
Caelo	Ácido tartárico	19825005	1
Caelo	Ácido tartárico	21000301001	2
Caelo	Ácido tartárico	21000938002	3
Caelo	Ácido tartárico	21000938004	1
Caelo	Ácido tartárico	21000938006	1
Caelo	Ácido tartárico	21000938007	2
Caelo	Ácido tartárico	21000938008	1
Caelo	Ácido tartárico	21002221001	1
Caelo	Ácido tartárico	2717I-01053	1
Caelo	Ácido tartárico	4110N-01053	1
Caelo	Ácido tartárico	708061	2
Caelo	Ácido tartárico	8051809	1
Caelo	Ácido tartárico	9041703	1
Caelo	Ácido tartárico	9494239	1
Caesar & Loretz GmbH...	Ácido tartárico	17337504	2
Caesar & Loretz GmbH...	Ácido tartárico	18239405	1
Caesar & Loretz GmbH...	Ácido tartárico	18121211	1
Caesar & Loretz GmbH...	Ácido tartárico	191825003	1
Caesar & Loretz GmbH/Gehe	Ácido tartárico	18121211	1
Caesar & Loretz GmbH/Gehe	Ácido tartárico	18121214	1
Caesar & Loretz GmbH/Gehe	Ácido tartárico	191825002	3
Caesar & Loretz GmbH/Gehe	Ácido tartárico	9494222	1
Caesar & Loretz GmbH...	Ácido tartárico	191825004	1
Caesar & Loretz GmbH...	Ácido tartárico	182394004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Ácido tartárico	18239405	1
Caesar & Loretz GmbH...	Ácido tartárico	17337505	1
Caesar & Loretz GmbH...	Ácido tartárico	18121212	1
Caesar & Loretz GmbH	Ácido tartárico	18121204	1
Caesar & Loretz GmbH	Ácido tartárico	18121208	3
Caesar & Loretz GmbH	Ácido tartárico	18121210	1
Caesar & Loretz GmbH	Ácido tartárico	18121211	1
Caesar & Loretz GmbH	Ácido tartárico	18239405	1
Caesar & Loretz GmbH	Ácido tartárico	18239406	1
Caesar & Loretz GmbH	Ácido tartárico	191825002	3
Caesar & Loretz GmbH	Ácido tartárico	191825003	7
Caesar & Loretz GmbH	Ácido tartárico	191825004	3
Caesar & Loretz GmbH	Ácido tartárico	191825005	2
Caesar & Loretz GmbH	Ácido tartárico	19182501	1
Caesar & Loretz GmbH	Ácido tartárico	21000938003	3
Caesar & Loretz/ Noweda	Ácido tartárico	12044103	1
canea, anzag	Ácido tartárico	12286906	1
Distillerie Mazzari/...	Ácido tartárico	13405	1
E-plus	Ácido tartárico	15349107	1
Euro OTC	Ácido tartárico	1604046-02	1
Euro OTC	Ácido tartárico	17347103	1
Euro OTC	Ácido tartárico	702265	1
Fagron	Ácido tartárico	1106211053	1
Fagron	Ácido tartárico	11E24-N06	1
Fagron	Ácido tartárico	11E24-N060752/764	1
Fagron	Ácido tartárico	12131	2
Fagron	Ácido tartárico	12225	1
Fagron	Ácido tartárico	12F18-N02	1
Fagron	Ácido tartárico	12F18-No2	1
Fagron	Ácido tartárico	12H02-N07	3
Fagron	Ácido tartárico	12K16-N02	1
Fagron	Ácido tartárico	12K29-B01-285247	1
Fagron	Ácido tartárico	13/25-B01	1
Fagron	Ácido tartárico	13/25-B01-285487	1
Fagron	Ácido tartárico	13/25-B01-285488	2
Fagron	Ácido tartárico	13/25-B01-294094	1
Fagron	Ácido tartárico	1325-B01-294093	1
Fagron	Ácido tartárico	1325-B01-294094	1
Fagron	Ácido tartárico	13B15N01	1
Fagron	Ácido tartárico	13B15-N01	8
Fagron	Ácido tartárico	13G03-N14	1
Fagron	Ácido tartárico	13I25-B01	1
Fagron	Ácido tartárico	13I25-B01-285487	1
Fagron	Ácido tartárico	13I25-B01-285488	2
Fagron	Ácido tartárico	13I25-b01-294093	1
Fagron	Ácido tartárico	13I25-B01-294093	3
Fagron	Ácido tartárico	13I25-B01-294094	5
Fagron	Ácido tartárico	13I25-B01-294095	1
Fagron	Ácido tartárico	13l25-B01-285488	1
Fagron	Ácido tartárico	14186212	1
Fagron	Ácido tartárico	14519	1
Fagron	Ácido tartárico	14G07-802	1
Fagron	Ácido tartárico	14G07-B02	3
Fagron	Ácido tartárico	14G07-B02-308554	3
Fagron	Ácido tartárico	14G07-B02-308555	2
Fagron	Ácido tartárico	14G07-B02-322976	2
Fagron	Ácido tartárico	14G07-B02-322977	1
Fagron	Ácido tartárico	14G07-B02-330640	4
Fagron	Ácido tartárico	15045303	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ácido tartárico	18G17-B01-351824	1
Fagron	Ácido tartárico	20151112-2	1
Fagron	Ácido tartárico	20A17-B04-196364	1
Fagron	Ácido tartárico	20A17-B04-200531	1
Fagron	Ácido tartárico	20A17-B04-200532	2
Fagron	Ácido tartárico	20J05-B01-202753	1
Fagron	Ácido tartárico	2414E1053	1
Fagron	Ácido tartárico	2513M01053	1
Fagron	Ácido tartárico	B04-2005302	1
Fagron	Ácido tartárico	P161019AT09/18	1
Fagron	Ácido tartárico	xxxxxxx	1
fischar, Gehe	Ácido tartárico	700061	1
Fischar/Gehe	Ácido tartárico	705061	1
Fischar/PH	Ácido tartárico	700061	1
Fischar/Phönix 05.07...	Ácido tartárico	700061	1
Fischar/Phönix	Ácido tartárico	704021	1
Fischar	Ácido tartárico	704061	2
Fischar	Ácido tartárico	705061	1
Fischar	Ácido tartárico	709041	1
Fischer/AHD	Ácido tartárico	700061	1
Fragon/Sanacorp	Ácido tartárico	13G03-N14	2
Gatt-Koller / Phoenix	Ácido tartárico	3334/08131514	1
GEHE 14.04.2014	Ácido tartárico	12H02-N07	1
GEHE 14.04.2014	Ácido tartárico	13G03-N14	2
Gehe/Fischer	Ácido tartárico	706061	1
Gehe/Henry Lamotte	Ácido tartárico	17/12	1
Gehe	Ácido tartárico	1325-B01-285487	1
Gehe	Ácido tartárico	16146806	1
Gehe	Ácido tartárico	191825002	2
Gehe	Ácido tartárico	21000938008	1
Gehe	Ácido tartárico	703061	1
Gehe	Ácido tartárico	7284696	1
Hänseler	Ácido tartárico		1
Klenk	Ácido tartárico	13405	1
L12	Ácido tartárico	14G07-B02-308555	1
Nachprüfung	Ácido tartárico	2082019-13	1
Noweda 20.7.19	Ácido tartárico	18121212	1
Noweda/ Fischar	Ácido tartárico	702061	1
Noweda	Ácido tartárico	7284696	1
Otto Fischar/ Gehe	Ácido tartárico	709041	1
Otto Fischar	Ácido tartárico	705061	2
Otto Fischer GmbH	Ácido tartárico	705061	1
Phoenix	Ácido tartárico	12044115	1
Phoenix	Ácido tartárico	12Ho2-N07	1
Phoenix	Ácido tartárico	12K29B01	1
Phoenix	Ácido tartárico	13116308	1
Phönix Gotha	Ácido tartárico	704021	1
Phönix	Ácido tartárico	11e24-n06	1
Phönix	Ácido tartárico	12286904	1
Phönix	Ácido tartárico	13/25-B01-294094	1
Phönix	Ácido tartárico	18121208	1
Sanacorp WE: 19.0518...	Ácido tartárico	16260406	1
Sanacorp	Ácido tartárico	17347104	2
Sanacorp	Ácido tartárico	191825005	2
Sanacorp	Ácido tartárico	21000301006	1
Sanacorp	Ácido tartárico	23000312004	1
schubert / Phoenix	Ácido tartárico	1014PLV-755	1
Spangropharm	Ácido tartárico	10073111	1

- 235 627 spectra from 1515 *Apo-Ident* customers from a total of 49 081 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido tartárico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido tartárico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	510	0	152 452
Type B	0	190	0	201 894
Type C	0	440	0	235 627

The substance/substance group *Ácido tartárico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6364 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22383	22613	8,64	218,33
22384	22384	0,00	215,47
22391	22391	0,00	218,71
22501	22391	3,76	220,33
22613	22613	0,00	221,02
24806	24806	0,00	217,46
25628	25628	0,00	222,78
25699	25699	0,00	222,49
26397	22391	5,41	222,57
27307	27307	0,00	227,30

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido tranexâmico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20397-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido tranexâmico; Acidum tranexamicum

Special notes

When selecting the *Ácido tranexâmico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido tranexâmico	9	4	43

Second-stage model

For differentiation of the substance/substance group *Ácido tranexâmico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido tranexâmico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	83,84	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido tranexâmico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido tranexâmico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Ácido tranexâmico	APX1508016MT	23504	40	20170224
Audor Pharma	Ácido tranexâmico	APX1803027MT	24708	40	20180430
Euro OTC	Ácido tranexâmico	2002005	25078	40	20200219*
Euro OTC	Ácido tranexâmico	2001034	25099	40	20200218*
Euro OTC	Ácido tranexâmico	2304017	26652	40	20230508*
Euro OTC	Ácido tranexâmico	2304017	26652SI	20	20230508*
Euro OTC	Ácido tranexâmico	2312001	27140	40	20240313*
Euro OTC	Ácido tranexâmico	2312001	27140SI	20	20240313*
Fagron	Ácido tranexâmico	14C21-B08-292225	21654	60	AR-17-FG-016394-01
Fagron	Ácido tranexâmico	14L15-B06-3000036	21727	60	AR-15-FG-008937-02
Fagron	Ácido tranexâmico	20H24-F02-373687	25586	40	20200923

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Ácido tranexâmico*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 522 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Ácido tranexâmico*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ácido tranexâmico	2006030	25247	40
Euro OTC	Ácido tranexâmico	2203031	26098	40
Fagron	Ácido tranexâmico	16E31-B07-331591	23503	50
Fagron	Ácido tranexâmico	21B05-F03-377271	25745	50
Euro OTC	Ácido tranexâmico	2203031	26098SI	20
Fagron	Ácido tranexâmico	16E31-B07-331591	23505	40

- 201 844 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 102 spectra from 70 *Apo-Ident* customers from 49 batches from the substance/substance group *Ácido tranexâmico*.

- Among them are spectra of independent samples from 43 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ácido tranexâmico	21B05-F03-377271	2
	Ácido tranexâmico	2304017-01	4
	Ácido tranexâmico	2312001-01	1
AHD	Ácido tranexâmico	APX1712011MT	2
Audor Pharma	Ácido tranexâmico	1508016MT	1
Audor Pharma	Ácido tranexâmico	APX1508016MT	4
Audor Pharma	Ácido tranexâmico	APX1611013MT	6
Audor Pharma	Ácido tranexâmico	APX17112011MT	1
Audor Pharma	Ácido tranexâmico	APX1712011MT	8
Audor Pharma	Ácido tranexâmico	ApX1803027MT	1
Audor Pharma	Ácido tranexâmico	APX1803027MT	6
Audor Pharma	Ácido tranexâmico	X1611013M	2
Audor Pharma	Ácido tranexâmico	X1706014M	1
Audor Pharma	Ácido tranexâmico	X1712011M	1
Audor Pharma	Ácido tranexâmico	X1803027M	1
Caelo	Ácido tranexâmico	15J29-B04	1
Caelo	Ácido tranexâmico	16E31-B07-331591	1
Caelo	Ácido tranexâmico	18/25-B05-354991	1
Caelo	Ácido tranexâmico	18A17-B05-345037	1
Caelo	Ácido tranexâmico	2006030-02	1
Caelo	Ácido tranexâmico	APX1712011MT	1
Euro OTC	Ácido tranexâmico		1
Euro OTC	Ácido tranexâmico	2002005-01	1
Euro OTC	Ácido tranexâmico	2006030-01	11
Euro OTC	Ácido tranexâmico	2006030-02	1
Euro OTC	Ácido tranexâmico	2203031-01	1
Euro OTC	Ácido tranexâmico	TXAA200005	1
Fagron	Ácido tranexâmico	1197-18-8	1
Fagron	Ácido tranexâmico	12D11-N02	1
Fagron	Ácido tranexâmico	13D08-N24	1
Fagron	Ácido tranexâmico	13D08-N240002/40	1
Fagron	Ácido tranexâmico	13Do8-N24	1
Fagron	Ácido tranexâmico	13G24-N21	1
Fagron	Ácido tranexâmico	13K08-B04-287966	1
Fagron	Ácido tranexâmico	15J29-B04	1
Fagron	Ácido tranexâmico	15J29-B04-312372	1
Fagron	Ácido tranexâmico	16B03-B02-319617	2
Fagron	Ácido tranexâmico	16J29-B04-312372	1
Fagron	Ácido tranexâmico	18A17-B05-345037	1
Fagron	Ácido tranexâmico	18A17-B05-345038	1
Fagron	Ácido tranexâmico	18F20-B01	1
Fagron	Ácido tranexâmico	18F20-B01-351691	3
Fagron	Ácido tranexâmico	18F20-B01-351693	1
Fagron	Ácido tranexâmico	18J25-B05	1
Fagron	Ácido tranexâmico	18J25-B05-354991	4
Fagron	Ácido tranexâmico	20H24-F02	1
Fagron	Ácido tranexâmico	20H24F02373687	1
Fagron	Ácido tranexâmico	20H24-F02-373687	2
Fagron	Ácido tranexâmico	21B05-F03-377271	2
Fagron	Ácido tranexâmico	5041804	1
Fagron	Ácido tranexâmico	F02-3736807	1
Fagron	Ácido tranexâmico	X1712011M	1
Fagron	Ácido tranexâmico	X19D25-B01-361249	1
Fagron	Ácido tranexâmico	X2012306M	1
Noweda	Ácido tranexâmico	18a17-b05-345037	1
Sanacorp	Ácido tranexâmico	16E31-B07-331591	1
Sanacorp	Ácido tranexâmico	2002005-02	1
Sanacorp	Ácido tranexâmico	2006030-01	1

- 235 965 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido tranexâmico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido tranexâmico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	240	0	201 844
Type C	0	102	0	235 965

The substance/substance group *Ácido tranexâmico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 94.1176 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21654	21654	0,00	119,50
21727	21727	0,00	112,39
23504	25099	4,08	111,52
24708	25099	4,34	117,14
25078	25078	0,00	109,47
25099	25099	0,00	114,59
25586	25078	9,32	119,17
26652	26652	0,00	118,93
27140	27140	0,00	121,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ácido ursodeoxicólico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006311-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ácido ursodeoxicólico; Ácido Ursodesoxicólico; Ursodiol

Special notes

When selecting the *Ácido ursodeoxicólico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ácido ursodeoxicólico	4	3	0

Second-stage model

For differentiation of the substance/substance group *Ácido ursodeoxicólico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ácido ursodeoxicólico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	81,55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ácido ursodeoxicólico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ácido ursodeoxicólico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ácido ursodeoxicólico	20F18-F22-372321	26471	40	240603341
Fagron	Ácido ursodeoxicólico	22C09-B03-223073	26472	40	20220526
Fagron	Ácido ursodeoxicólico	23E29-B08-228646	26902	40	20230704
Fagron	Ácido ursodeoxicólico	23E29-B08-228646	26902SI	20	20230704
Fagron	Ácido Ursodesoxicólico	UDCA-II-20240633	BR20032	40	20240709*
Fagron	Ácido Ursodesoxicólico	UDCA-II-20240633	BR20032SI	20	20240709*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 200 spectra of 6 reference samples from the substance/substance group *Ácido ursodeoxicólico*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 762 spectra from a total of 2838 batches from further 484 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 7 reference samples from the substance/substance group *Ácido ursodeoxicólico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ácido ursodeoxicólico	24C07-B17-236823	27265	40
Fagron	Ácido Ursodesoxicólico	UDCA-II-20240807	BR20033	40
Fagron	Ácido Ursodesoxicólico	UDCA-II-20240312	BR20034	40
Fagron	Ácido ursodeoxicólico	20F18-F22-372321	26471SI†	20
Fagron	Ácido ursodeoxicólico	22C09-B03-223073	26472SI†	20
Fagron	Ácido Ursodesoxicólico	UDCA-II-20240807	BR20033SI	20
Fagron	Ácido Ursodesoxicólico	UDCA-II-20240312	BR20034SI	20

- 201 884 spectra from a total of 4040 batches from further 841 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ácido ursodeoxicólico*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ácido ursodeoxicólico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ácido ursodeoxicólico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	200	0	201 884
Type C	0	0	0	236 067

The substance/substance group *Ácido ursodeoxicólico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26471	26471	0,00	149,63
26472	26471	53,49	145,85
26902	26471	54,01	145,41
BR20032	BR20032	0,00	142,23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Alantoína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20079-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Alantoína; Allantoinum

Special notes

When selecting the *Alantoína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Alantoína	7	7	123

Second-stage model

For differentiation of the substance/substance group *Alantoína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Alantoína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	110,92	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Alantoína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Alantoína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Alantoína	162289	22756	40	20160815*
Caelo	Alantoína	172346	23629	40	20171019*
Caelo	Alantoína	172346	23635	40	20171019*
Euro OTC	Alantoína	1406011-01	21625	60	20140718
Euro OTC	Alantoína	1609012	22750	40	20161006*
Euro OTC	Alantoína	1609012-01	22810	40	20161006
Euro OTC	Alantoína	1406011-04	24095	40	20170213
Fagron	Alantoína	13I03-B05	21216	40	20130927

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 340 spectra of 8 reference samples from the substance/substance group *Alantoína*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 330 spectra of 9 reference samples from the substance/substance group *Alantoína*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Alantoína	181586	24235	40
Caelo	Alantoína	191828	24894	40
Caelo	Alantoína	21003135	25848	50
Caelo	Alantoína	23000841	27337	40
Euro OTC	Alantoína	1811006	24344	40
Euro OTC	Alantoína	2101022	25593	40
Euro OTC	Alantoína	2212010	26511	40
Caelo	Alantoína	23000841	27337SI	20
Euro OTC	Alantoína	2212010	26511SI	20

- 201 754 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 564 spectra from 256 *Apo-Ident* customers from 126 batches from the substance/substance group *Alantoína*.

- Among them are spectra of independent samples from 123 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Alantoína	20004526005	1
	Alantoína	21003135003	1
	Alantoína	21003135007	1
	Alantoína	21003135015	1
ACM Herba	Alantoína	22J00443	1
AHD	Alantoína	1609012-01	1
Anzag;18.03.15;2,76EUR	Alantoína	14247602	1
Caelo	Alantoína	10064008	4
Caelo	Alantoína	10064012	1
Caelo	Alantoína	10064015	1
Caelo	Alantoína	10318305	1
Caelo	Alantoína	10318312	1
Caelo	Alantoína	10318313	2
Caelo	Alantoína	1113E-01087	1
Caelo	Alantoína	11247504	5
Caelo	Alantoína	11247510	2
Caelo	Alantoína	11247511	2
Caelo	Alantoína	121127	1
Caelo	Alantoína	1225101	1
Caelo	Alantoína	12251501	4
Caelo	Alantoína	12251502	2
Caelo	Alantoína	12251505	7
Caelo	Alantoína	12251510	9
Caelo	Alantoína	12251511	1
Caelo	Alantoína	12374401	1
Caelo	Alantoína	12374403	8
Caelo	Alantoína	12374404	2
Caelo	Alantoína	12374407	4
Caelo	Alantoína	12374408	1
Caelo	Alantoína	12374409	15
Caelo	Alantoína	12374414	8
Caelo	Alantoína	12374415	10
Caelo	Alantoína	12374417	1
Caelo	Alantoína	12374418	2
Caelo	Alantoína	12374422	9
Caelo	Alantoína	12374423	2
Caelo	Alantoína	1251505	1
Caelo	Alantoína	140512	1
Caelo	Alantoína	1406011-05	1
Caelo	Alantoína	14247602	6
Caelo	Alantoína	14247609	10
Caelo	Alantoína	14247610	1
Caelo	Alantoína	1522000	1
Caelo	Alantoína	152200012	1
Caelo	Alantoína	15220004	1
Caelo	Alantoína	15220005	2
Caelo	Alantoína	15220006	17
Caelo	Alantoína	15220007	4
Caelo	Alantoína	15220008	11
Caelo	Alantoína	15220010	3
Caelo	Alantoína	15220011	2
Caelo	Alantoína	15220012	11
Caelo	Alantoína	1522008	1
Caelo	Alantoína	15275302	1
Caelo	Alantoína	15275304	3
Caelo	Alantoína	15275305	3
Caelo	Alantoína	15275312	8
Caelo	Alantoína	16228903	13
Caelo	Alantoína	16228904	1
Caelo	Alantoína	16228906	17

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alantoína	16228913	2
Caelo	Alantoína	16228914	3
Caelo	Alantoína	16228915	28
Caelo	Alantoína	17355901	2
Caelo	Alantoína	17355903	20
Caelo	Alantoína	17355904	1
Caelo	Alantoína	17355905	1
Caelo	Alantoína	1811006-01	1
Caelo	Alantoína	18158602	12
Caelo	Alantoína	18158604	12
Caelo	Alantoína	18158605	4
Caelo	Alantoína	18158606	1
Caelo	Alantoína	18158613	3
Caelo	Alantoína	1918202	1
Caelo	Alantoína	191828002	2
Caelo	Alantoína	19182802	1
Caelo	Alantoína	19182803	7
Caelo	Alantoína	20002009004	7
Caelo	Alantoína	20004518002	3
Caelo	Alantoína	20004518003	8
Caelo	Alantoína	20004526003	7
Caelo	Alantoína	20004526005	5
Caelo	Alantoína	20004526006	1
Caelo	Alantoína	2004526005	1
Caelo	Alantoína	20071202	1
Caelo	Alantoína	20140612-15	1
Caelo	Alantoína	21003135003	1
Caelo	Alantoína	21003135007	5
Caelo	Alantoína	2100315007	1
Caelo	Alantoína	2264594	1
Caelo	Alantoína	2713431	1
Caelo	Alantoína	2713448	1
Caelo	Alantoína	28101702	1
Caelo	Alantoína	4247602	1
Caelo	Alantoína	5051402	1
Caelo	Alantoína	81542099	1
Caelo	Alantoína	81542358	2
Caesar & Loretz GmbH...	Alantoína	17355905	2
Caesar & Loretz GmbH...	Alantoína	191828002	1
Caesar & Loretz GmbH...	Alantoína	18158605	1
Caesar & Loretz GmbH...	Alantoína	191828002	1
Caesar & Loretz GmbH...	Alantoína	20002009004	1
Caesar & Loretz GmbH...	Alantoína	18158604	2
Caesar & Loretz GmbH...	Alantoína	20002009004	1
Caesar & Loretz GmbH...	Alantoína	18158604	1
Caesar & Loretz GmbH	Alantoína	12251505	1
Caesar & Loretz GmbH	Alantoína	12251510	1
Caesar & Loretz GmbH	Alantoína	12374403	1
Caesar & Loretz GmbH	Alantoína	12374409	1
Caesar & Loretz GmbH	Alantoína	12374415	1
Caesar & Loretz GmbH	Alantoína	12374416	1
Caesar & Loretz GmbH	Alantoína	14247602	1
Caesar & Loretz GmbH	Alantoína	18158602	2
Caesar & Loretz GmbH	Alantoína	18158604	3
Caesar & Loretz GmbH	Alantoína	18158605	1
Caesar & Loretz GmbH	Alantoína	18158613	2
Caesar & Loretz GmbH	Alantoína	191828002	4
Caesar & Loretz GmbH	Alantoína	19182803	4
Caesar & Loretz GmbH	Alantoína	20004518002	1
Caesar & Loretz GmbH	Alantoína	20004518003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
CAESAR & LORETZ GMBH	Alantoína	20004526005	1
Caesar & Loretz GmbH	Alantoína	21003135007	1
Caesar & Loretz Hilden	Alantoína	17355903	1
Caesar & Loretz	Alantoína	16228906	1
Caesar&Loretz GmbH	Alantoína	12374409	1
Caeser / Gehe	Alantoína	15220007	1
Cealo/Phönix	Alantoína	18158602	1
celo/Jenne	Alantoína	12374403	1
Deretil SA / Allianc...	Alantoína	2101022-01	1
DSM Nutritional Prod...	Alantoína	12251505	1
EuRho / Phoenix	Alantoína	1406011-03	1
EuRho	Alantoína	1406011-04	1
Euro OTC	Alantoína	140104601	1
Euro OTC	Alantoína	1401046-01	3
Euro OTC	Alantoína	1406011	2
Euro OTC	Alantoína	1406011-01	7
Euro OTC	Alantoína	1406011-02	3
Euro OTC	Alantoína	140601103	1
Euro OTC	Alantoína	1406011-04	1
Euro OTC	Alantoína	1406011-05	3
Euro OTC	Alantoína	15220008	2
Euro OTC	Alantoína	1609012-01	10
Euro OTC	Alantoína	160901202	1
Euro OTC	Alantoína	1609012-02	3
Euro OTC	Alantoína	1609012-03	2
Euro OTC	Alantoína	16228915	1
Euro OTC	Alantoína	18110006-01	1
Euro OTC	Alantoína	1811006	1
Euro OTC	Alantoína	1811006-01	11
Euro OTC	Alantoína	181100602	1
Euro OTC	Alantoína	1811006-02	11
Euro OTC	Alantoína	1811006-03	8
Euro OTC	Alantoína	2101022-01	8
Euro OTC	Alantoína	5024-000077	1
Euro OTC	Alantoína	K93504015	1
Fagron	Alantoína	11J11-N11	3
Fagron	Alantoína	12B09-N09	1
Fagron	Alantoína	12C30-N04	1
Fagron	Alantoína	13A21-N07	3
Fagron	Alantoína	13G16-N07	6
Fagron	Alantoína	13I03-B05-289430	1
Fagron	Alantoína	16228905	2
Fagron	Alantoína	5011E-01087	1
Fargron/AHD	Alantoína	13G16-N07	1
Gehe	Alantoína	12251510	1
Gehe	Alantoína	14247603	1
Gehe	Alantoína	15220008	1
Gehe	Alantoína	15220012	1
Gehe	Alantoína	1609012-02	1
Gehe	Alantoína	17355903	1
Gehe	Alantoína	1811006-02	1
Herba Chemosan	Alantoína	22JOD443	1
Ichthyol-Gesellschaft	Alantoína	16228915	1
Kehr	Alantoína	15220008	1
Krieger/Hedinger	Alantoína	15220006	1
Merck	Alantoína	1406011-05	1
Merck	Alantoína	160901201	1
Merck	Alantoína	1609012-01	1
Noweda	Alantoína	1609012-01	1
Noweda	Alantoína	16228915	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Alantoína	21003135015	1
Noweda	Alantoína	2101022-02	1
Phoenix 08.10.14	Alantoína	1401046-01	1
Sanacorp	Alantoína	12251501	1
Sanacorp	Alantoína	12251510	1
Sanacorp	Alantoína	12374409	2
Sanacorp	Alantoína	12374422	1
Sanacorp	Alantoína	15275312	1
Sanacorp	Alantoína	1811006-02	1
Sanacorp	Alantoína	K93504015	1
Spinnrad	Alantoína	1217503012	1
VDL 17.10.14	Alantoína	12374415	1

- 235 503 spectra from 1515 *Apo-Ident* customers from a total of 49 132 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Alantoína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Alantoína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	330	0	201 754
Type C	0	562	2	235 503

The substance/substance group *Alantoína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1818 %)
Type C	100.0000 % (> 99.9007 %)	99.6454 % (> 99.1135 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21216	22756	10,19	288,39
21625	22750	9,93	288,78
22750	22750	0,00	283,25
22756	22756	0,00	276,82
22810	22750	6,04	278,41
23629	23629	0,00	274,08
23635	23635	0,00	275,83
24095	22750	6,28	281,58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Albendazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21596-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Albendazol; Albendazolum

Special notes

When selecting the *Albendazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Albendazol	6	3	14

Second-stage model

For differentiation of the substance/substance group *Albendazol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Albendazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de clonidina	165,58	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Albendazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Albendazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Albendazol	2208010	26263	40	20220831*
Euro OTC	Albendazol	2208010	26263SI	20	20220831*
Fagron	Albendazol	12J25-B40-293217	21596	45	AR-15-FG-002571-01
Fagron	Albendazol	16B04-B06-329519	23017	40	20160302
Fagron	Albendazol	18C21-B04-351586	24578	40	20180625
Fagron	Albendazol	20B27-F01-373154	25714	40	20200901
Fagron	Albendazol	22B26-B05-219216	26174	40	20220602

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 265 spectra of 7 reference samples from the substance/substance group *Albendazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 697 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Albendazol*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Albendazol	14B05-B41-299704	21730	60
Fagron	Albendazol	14B05-B41-314321	22940	40
Fagron	Albendazol	16B04-B06-322057	22968	40
Fagron	Albendazol	22B26-B05-219216	26174SI†	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 28 spectra from 14 *Apo-Ident* customers from 17 batches from the substance/substance group *Albendazol*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Fagron	Albendazol	14B05-B41	1
Fagron	Albendazol	14B05-B41-305249	1
Fagron	Albendazol	14B05B41-312959	1
Fagron	Albendazol	14B05-B41-312959	1
Fagron	Albendazol	14b05-b41-314321	1
Fagron	Albendazol	14B05-B41-314321	1
Fagron	Albendazol	16B04-B06-322055	2
Fagron	Albendazol	16B04-B06-329519	1
Fagron	Albendazol	16B04-B06-337998	2
Fagron	Albendazol	18C21-B04	1
Fagron	Albendazol	18C21-B04-350057	1
Fagron	Albendazol	18C21-B04-351584	1
Fagron	Albendazol	18C21-B04-351585	3
Fagron	Albendazol	18C21-B04-351586	4
Fagron	Albendazol	18C21-B04-357034	1
Fagron	Albendazol	18C21-B04x3	1
Fagron	Albendazol	20B27-F01-373151	5

- 236 039 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Albendazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Albendazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	265	0	152 697
Type B	0	160	0	201 924
Type C	0	28	0	236 039

The substance/substance group *Albendazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7358 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 78.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21596	21596	0,00	287,83
23017	26263	16,75	296,36
24578	26263	13,40	306,22
25714	26263	12,33	302,73
26174	26263	9,13	302,86
26263	26263	0,00	303,66

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Álcoois de cera de lã**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20495-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Álcoois de cera de lã; Alcoholes lanae

Special notes

When selecting the *Álcoois de cera de lã* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Álcoois de cera de lã	6	2	21

Second-stage model

For differentiation of the substance/substance group *Álcoois de cera de lã* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Álcoois de cera de lã* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Monoestearato de glicerol, emulsionante	74,88	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Álcoois de cera de lã* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Álcoois de cera de lã*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Álcoois de cera de lã	13380601	21520	40	1412037
Caelo	Álcoois de cera de lã	153703	22328	60	20151111*
Caelo	Álcoois de cera de lã	153703	22329	60	20151111*
Caelo	Álcoois de cera de lã	163530	23098	40	20161223*
Caelo	Álcoois de cera de lã	191275	24722	40	20190606*
Caelo	Álcoois de cera de lã	22002307001	26302	40	20220805
Caelo	Álcoois de cera de lã	22002307001	26302SI	20	20220805
Caelo	Álcoois de cera de lã	24002633	27419	40	20241125*
Caelo	Álcoois de cera de lã	24002633	27419SI	20	20241125*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Álcoois de cera de lã*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 602 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Álcoois de cera de lã*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Álcoois de cera de lã	173160	23972	40
Caelo	Álcoois de cera de lã	181619	24165	40

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 35 spectra from 22 *Apo-Ident* customers from 22 batches from the substance/substance group *Álcoois de cera de lã*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Álcoois de cera de lã	11011401	1
Caelo	Álcoois de cera de lã	12340505	1
Caelo	Álcoois de cera de lã	13071502	1
Caelo	Álcoois de cera de lã	13083906	2
Caelo	Álcoois de cera de lã	13083912	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Álcoois de cera de lã	13226408	1
Caelo	Álcoois de cera de lã	13380601	1
Caelo	Álcoois de cera de lã	14262501	1
Caelo	Álcoois de cera de lã	15304502	1
Caelo	Álcoois de cera de lã	15304505	3
Caelo	Álcoois de cera de lã	17169701	3
Caelo	Álcoois de cera de lã	18092502	3
Caelo	Álcoois de cera de lã	18161904	1
Caelo	Álcoois de cera de lã	18161912	1
Caelo	Álcoois de cera de lã	19127504	2
Caelo	Álcoois de cera de lã	20002460003	1
Caelo	Álcoois de cera de lã	21002143004	1
Caelo	Álcoois de cera de lã	23101408	1
Caelo	Álcoois de cera de lã	4/2015	1
Caelo	Álcoois de cera de lã	6111801	1
Caesar & Loretz GmbH…	Álcoois de cera de lã	20002460003	1
Caesar & Loretz GmbH	Álcoois de cera de lã	18161904	1
Caesar & Loretz GmbH	Álcoois de cera de lã	19127504	1
Caesar & Loretz GmbH	Álcoois de cera de lã	20002460003	1
Cealo/ Noweda	Álcoois de cera de lã	13380601	1
Fagron	Álcoois de cera de lã	16235702	1
Noweda	Álcoois de cera de lã	22002784004	1

- 236 032 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Álcoois de cera de lã* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Álcoois de cera de lã* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	80	0	202 004
Type C	0	34	1	236 032

The substance/substance group *Álcoois de cera de lã* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	97.1429 % (> 88.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21520	21520	0,00	117,56
22328	22328	0,00	128,39
22329	22329	0,00	127,64
23098	23098	0,00	120,25
24722	24722	0,00	128,50
26302	24722	19,00	125,58
27419	27419	0,00	127,87

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Álcool cetoestearílico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20738-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Álcool cetoestearílico; Alcohol cetylicus; Alcohol cetylicus et stearylicus; Álcool cetilestearílico; Álcool cetílico; Álcool cetoestearílico (tipo A), emuls; Cetearyl Alcohol (and) Ceteareth-20 (base autoemulsionável não-iônica); Cetostearyl alcohol (type A), emulsifying; Emulgade® 1000 NI

Special notes

When selecting the *Álcool cetoestearílico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Álcool cetoestearílico	34	25	473

Second-stage model

For differentiation of the substance/substance group *Álcool cetoestearílico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Álcool cetoestearílico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Álcool emulsificante não iônico	20,37	–
Monoestearato de glicerol, emulsionante	42,62	–
Monoestearato de glicerol 60	69,82	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Álcool cetoestearílico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Álcool cetoestearílico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Álcool cetilestearílico	14054504	21314	40	20140226
Caelo	Álcool cetilestearílico	14054504	21442	60	20140226
Caelo	Álcool cetilestearílico	17049205	23725	40	20170302
Caelo	Álcool cetilestearílico	20002898002	25499	40	20200916
Caelo	Álcool cetilestearílico	21003928003	26231	40	20211208
Caelo	Álcool cetilestearílico	23000403	26698	40	20230228*
Caelo	Álcool cetilestearílico	23002042	26941	40	20230922*
Caelo	Álcool cetilestearílico	23002042	26941SI	20	20230922*
Fagron	Álcool cetilestearílico	13C13-N13	20968	40	1402265
Caelo	Álcool cetílico	13096901	20896	40	1405179
Caelo	Álcool cetílico	13286502	21318	40	20130925
Caelo	Álcool cetílico	13286502	21435	60	20130925
Caelo	Álcool cetílico	15323301	22266	60	AR-16-FG-008835-01
Caelo	Álcool cetílico	161063	22398	40	20160420*
Caelo	Álcool cetílico	161063	22399	40	20160420*
Caelo	Álcool cetílico	161063	22400	40	20160420*
Caelo	Álcool cetílico	161063	22401	40	20160420*
Caelo	Álcool cetílico	161063	22402	40	20160420*
Caelo	Álcool cetílico	161063	22403	40	20160420*
Caelo	Álcool cetílico	20002637001	25498	40	20201009

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Álcool cetílico	22000377002	26586	40	20220308
Caelo	Álcool cetílico	22000377002	26586SI	20	20220308
Caelo	Álcool cetílico	23000249	26695	40	20230224*
Caelo	Álcool cetílico	23000249	26695SI	20	20230224*
Caelo	Álcool cetílico	23000130	26697	40	20230224*
Caelo	Álcool cetílico	23000130	26697SI	20	20230224*
Euro OTC	Álcool cetílico	1508014-01	22611	40	20150821
Bombastus	Cetostearyl alcohol (type…	21004319	26025	40	20211011
Caelo	Cetostearyl alcohol (type…	13233005	21319	30	1506057
Caelo	Cetostearyl alcohol (type…	13233005	21434	60	20130816
Caelo	Cetostearyl alcohol (type…	14322505	21830	60	20141031
Caelo	Cetostearyl alcohol (type…	153857	22331	60	20151202*
Caelo	Cetostearyl alcohol (type…	153857	22332	60	20151202*
Caelo	Cetostearyl alcohol (type…	153856	22333	60	20160210*
Caelo	Cetostearyl alcohol (type…	153856	22334	60	20160210*
Euro OTC	Cetostearyl alcohol (type…	1510043	21998	60	20151124*
Euro OTC	Cetostearyl alcohol (type…	1504010-01	22264	60	20150423
Euro OTC	Cetostearyl alcohol (type…	2002033	25253	40	20200617*
Euro OTC	Cetostearyl alcohol (type…	2012002	25528	40	20210104*
Fagron	Cetostearyl alcohol (type…	13L17-B05	21279	40	1505070
Fagron	Cetostearyl alcohol (type…	16I13-B01-326511	23022	40	20161024
Caelo	Emulgade® 1000 NI	14055001	21381	40	20140225
Caelo	Emulgade® 1000 NI	15277504	22390	40	20150828
Caelo	Emulgade® 1000 NI	20000858003	25519	40	20200330
Caelo	Emulgade® 1000 NI	21002092004	25978	35	2208569
Caelo	Emulgade® 1000 NI	22002953003	26744	40	20221012
Caelo	Emulgade® 1000 NI	22002953003	26744SI	20	20221012
Fagron	Emulgade® 1000 NI	12H07-N06	20738	40	20120905
Fagron	Emulgade® 1000 NI	13C05-B40-289262	21054	40	1408003

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2065 spectra of 49 reference samples from the substance/substance group *Álcool cetoestearílico*. These samples are listed above in the *calibration samples* section. The reference samples come from 34 different batches.
- 150 897 spectra from a total of 2808 batches from further 482 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type B spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1260 spectra of 34 reference samples from the substance/substance group *Álcool cetoestearílico*.
- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Álcool cetilestearílico	170492	23097	40
Caelo	Álcool cetilestearílico	172979	23819	40
Caelo	Álcool cetilestearílico	190552	24721	40
Caelo	Álcool cetilestearílico	21000059005	25935	40
Caelo	Álcool cetilestearílico	24001586	27328	40
Caelo	Álcool cetílico	170473	23068	40
Caelo	Álcool cetílico	173155	23973	40
Caelo	Álcool cetílico	21001593	25697	50
Caelo	Álcool cetílico	23003036	27420	40
Caelo	Álcool cetílico	24002178	27421	40
Bombastus	Cetostearyl alcohol (type…	23004942	27060	40
Caelo	Cetostearyl alcohol (type…	171980	23575	40
Caelo	Cetostearyl alcohol (type…	180180	24033	40
Caelo	Cetostearyl alcohol (type…	191857	25068	40
Caelo	Cetostearyl alcohol (type…	20002023	25377	40
Caelo	Cetostearyl alcohol (type…	21000566	25663	40
Caelo	Cetostearyl alcohol (type…	22004149	26699	40
Caelo	Cetostearyl alcohol (type…	24002417	27417	40
Euro OTC	Cetostearyl alcohol (type…	1604013	22540	40
Euro OTC	Cetostearyl alcohol (type…	1701031	22999	40
Euro OTC	Cetostearyl alcohol (type…	1705001	23381	40
Euro OTC	Cetostearyl alcohol (type…	1711001	23737	40
Fagron	Cetostearyl alcohol (type…	23A11-B07-224497	26611	40
Fagron	Cetostearyl alcohol (type…	24G09-B04-003936	27470	40
Caelo	Emulgade® 1000 NI	160804	22395	40
Caelo	Álcool cetilestearílico	21003928003	26231SI†	20
Caelo	Álcool cetilestearílico	23000403	26698SI†	20
Bombastus	Cetostearyl alcohol (type…	23004942	27060SI	20
Caelo	Cetostearyl alcohol (type…	22004149	26699SI	20
Euro OTC	Cetostearyl alcohol (type…	1711001	25093	40
Fagron	Cetostearyl alcohol (type…	23A11-B07-224497	26611SI	20
Caelo	Emulgade® 1000 NI	160804	22396	40
Caelo	Emulgade® 1000 NI	160804	22397	40
Caelo	Emulgade® 1000 NI	21002092004	25978SI†	30

- 200 824 spectra from a total of 4017 batches from further 839 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1599 spectra from 607 *Apo-Ident* customers from 402 batches from the substance/substance group *Álcool cetoestearílico*.
- Among them are spectra of independent samples from 381 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Álcool cetilestearílico	1711001-02	1
	Cetostearyl alcohol (type…	2012002-02	1
	Álcool cetilestearílico	21000086001	2
	Cetostearyl alcohol (type…	21003223011	3
	Álcool cetílico	22000377002	1
	Emulgade® 1000 NI	22001170001	2
	Cetostearyl alcohol (type…	22001324007	1
	Cetostearyl alcohol (type…	22001329004	4
	Cetostearyl alcohol (type…	22001329007	1
	Cetostearyl alcohol (type…	22001329008	10
	Álcool cetilestearílico	22003074003	1
	Cetostearyl alcohol (type…	22004149004	2
	Cetostearyl alcohol (type…	2201329008	1
	Cetostearyl alcohol (type…	22C11-B02-222108	1
	Álcool cetílico	23000130003	1
	Álcool cetílico	23000130004	6
	Álcool cetílico	2300013004	1
	Álcool cetílico	23003036008	1
	Cetostearyl alcohol (type…	23A11-B07-224497	1
	Álcool cetílico	23E25-B05_230388	1
	Álcool cetílico	522202021	1
A.H.D.	Cetostearyl alcohol (type…	12L19-N03	2
ahd/lamotte	Álcool cetilestearílico	13210504	1
AHD	Álcool cetílico	17321603	1
AHD	Álcool cetílico	20002637001	1
AHD	Emulgade® 1000 NI	8073743	1
ALH	Cetostearyl alcohol (type…	15271405	1
Alliance Health 24.0…	Cetostearyl alcohol (type…	13L17-B05-289805	1
alliance health. 05.…	Cetostearyl alcohol (type…	14G31-B03-297610	1
Anzag	Cetostearyl alcohol (type…	12G02-N04	1
Audor Pharma	Cetostearyl alcohol (type…	16238602	1
BASF / Sanacorp	Cetostearyl alcohol (type…	B04-1953003	1
Bombastus	Cetostearyl alcohol (type…	18000081P-180824-1	1
Bombastus	Cetostearyl alcohol (type…	18000081P181203-4	1
Bombastus	Cetostearyl alcohol (type…	18000081P-190312-9	1
Bombastus	Cetostearyl alcohol (type…	18002312	3
Bombastus	Cetostearyl alcohol (type…	18003404	1
Bombastus	Cetostearyl alcohol (type…	18003437	4
Bombastus	Cetostearyl alcohol (type…	18006205P-190312-10	1
Bombastus	Cetostearyl alcohol (type…	19002555	5
Bombastus	Cetostearyl alcohol (type…	19005207P-200116-3	1
Bombastus	Cetostearyl alcohol (type…	19005208	2
Bombastus	Cetostearyl alcohol (type…	20001742	1
Bombastus	Cetostearyl alcohol (type…	20005694	2
Bombastus	Cetostearyl alcohol (type…	265360	1
Bombastus	Cetostearyl alcohol (type…	278418	1
Bombastus	Cetostearyl alcohol (type…	288691	3
Bombastus	Cetostearyl alcohol (type…	295148	2
Bombastus	Cetostearyl alcohol (type…	300132	5
Bombastus	Cetostearyl alcohol (type…	303935	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Cetostearyl alcohol (type…	308514	5
Bombastus	Cetostearyl alcohol (type…	60083112P-200326-4	1
Caelo	Cetostearyl alcohol (type…		3
Caelo	Cetostearyl alcohol (type…	11009204	1
Caelo	Álcool cetílico	1112013B	1
Caelo	Álcool cetílico	11153405	1
Caelo	Álcool cetilestearílico	11162305	1
Caelo	Cetostearyl alcohol (type…	11291101	1
Caelo	Cetostearyl alcohol (type…	11291103	1
Caelo	Álcool cetilestearílico	11302101	1
Caelo	Álcool cetílico	11320702	2
Caelo	Álcool cetílico	12018605	2
Caelo	Álcool cetilestearílico	12021304	1
Caelo	Álcool cetilestearílico	12025301	2
Caelo	Cetostearyl alcohol (type…	12065709	7
Caelo	Álcool cetílico	1212E-01076	1
Caelo	Cetostearyl alcohol (type…	12134203	1
Caelo	Cetostearyl alcohol (type…	12229402	2
Caelo	Cetostearyl alcohol (type…	12231402	1
Caelo	Álcool cetílico	12271103	5
Caelo	Cetostearyl alcohol (type…	12331402	7
Caelo	Cetostearyl alcohol (type…	12331407	3
Caelo	Álcool cetílico	12338604	6
Caelo	Cetostearyl alcohol (type…	12C30-N01	1
Caelo	Álcool cetilestearílico	13018305	4
Caelo	Álcool cetilestearílico	13018306	1
Caelo	Álcool cetílico	13096901	5
Caelo	Álcool cetílico	13096904	2
Caelo	Álcool cetilestearílico	1314405	1
Caelo	Cetostearyl alcohol (type…	13144103	1
Caelo	Cetostearyl alcohol (type…	13144104	2
Caelo	Cetostearyl alcohol (type…	13144105	12
Caelo	Cetostearyl alcohol (type…	13144107	2
Caelo	Álcool cetilestearílico	13206206	3
Caelo	Álcool cetílico	13210504	9
Caelo	Cetostearyl alcohol (type…	13233001	1
Caelo	Cetostearyl alcohol (type…	13233002	3
Caelo	Cetostearyl alcohol (type…	13233005	12
Caelo	Cetostearyl alcohol (type…	13233006	1
Caelo	Cetostearyl alcohol (type…	13233008	2
Caelo	Álcool cetílico	13286502	5
Caelo	Cetostearyl alcohol (type…	13352102	1
Caelo	Álcool cetilestearílico	13-B01-327355	1
Caelo	Cetostearyl alcohol (type…	13L17-B05-289806	1
Caelo	Álcool cetilestearílico	14054504	4
Caelo	Álcool cetilestearílico	14054508	3
Caelo	Emulgade® 1000 NI	14055002	1
Caelo	Álcool cetilestearílico	14061317	1
Caelo	Cetostearyl alcohol (type…	14156201	1
Caelo	Cetostearyl alcohol (type…	14158201	13
Caelo	Cetostearyl alcohol (type…	14158202	1
Caelo	Álcool cetilestearílico	14215007	6
Caelo	Álcool cetílico	14262204	5
Caelo	Cetostearyl alcohol (type…	14322502	2
Caelo	Cetostearyl alcohol (type…	14322505	12
Caelo	Cetostearyl alcohol (type…	14322506	2
Caelo	Cetostearyl alcohol (type…	14322512	1
Caelo	Álcool cetilestearílico	14346201	3
Caelo	Álcool cetilestearílico	14346202	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Álcool cetílico	14349101	14
Caelo	Cetostearyl alcohol (type…	14G31-B03-305612	3
Caelo	Cetostearyl alcohol (type…	15071704	1
Caelo	Cetostearyl alcohol (type…	15090701	10
Caelo	Cetostearyl alcohol (type…	15090703	2
Caelo	Cetostearyl alcohol (type…	15090706	3
Caelo	Cetostearyl alcohol (type…	1510043-01	1
Caelo	Emulgade® 1000 NI	15113703	1
Caelo	Álcool cetílico	1523316	1
Caelo	Cetostearyl alcohol (type…	15271402	9
Caelo	Cetostearyl alcohol (type…	15271403	9
Caelo	Cetostearyl alcohol (type…	15271405	12
Caelo	Cetostearyl alcohol (type…	15271407	9
Caelo	Cetostearyl alcohol (type…	15271408	3
Caelo	Cetostearyl alcohol (type…	15271410	1
Caelo	Álcool cetilestearílico	15272702	2
Caelo	Álcool cetilestearílico	15272709	6
Caelo	Álcool cetilestearílico	15272717	6
Caelo	Emulgade® 1000 NI	15277501	1
Caelo	Emulgade® 1000 NI	15277505	1
Caelo	Álcool cetílico	15323301	7
Caelo	Álcool cetílico	15323308	1
Caelo	Álcool cetílico	15323311	11
Caelo	Álcool cetílico	15323316	4
Caelo	Cetostearyl alcohol (type…	15385602	3
Caelo	Cetostearyl alcohol (type…	15385606	1
Caelo	Cetostearyl alcohol (type…	15789271	1
Caelo	Cetostearyl alcohol (type…	15C31-B99-307062	1
Caelo	Álcool cetilestearílico	16048812	3
Caelo	Emulgade® 1000 NI	16080403	1
Caelo	Emulgade® 1000 NI	16080407	2
Caelo	Álcool cetilestearílico	160914	1
Caelo	Álcool cetílico	16106307	4
Caelo	Cetostearyl alcohol (type…	16119604	14
Caelo	Cetostearyl alcohol (type…	16119607	2
Caelo	Álcool cetilestearílico	16230603	2
Caelo	Cetostearyl alcohol (type…	16238604	3
Caelo	Cetostearyl alcohol (type…	16238607	11
Caelo	Álcool cetílico	16335802	7
Caelo	Álcool cetílico	16335805	1
Caelo	Álcool cetílico	16335807	7
Caelo	Emulgade® 1000 NI	16348101	2
Caelo	Cetostearyl alcohol (type…	16I13-B01-327355	1
Caelo	Cetostearyl alcohol (type…	16I13-B01-327864	1
Caelo	Álcool cetílico	17047303	1
Caelo	Álcool cetílico	17047306	3
Caelo	Álcool cetílico	17047307	13
Caelo	Álcool cetilestearílico	17049209	2
Caelo	Álcool cetilestearílico	1705001-01	1
Caelo	Cetostearyl alcohol (type…	17056802	1
Caelo	Cetostearyl alcohol (type…	17056806	6
Caelo	Álcool cetilestearílico	1711001-02	2
Caelo	Álcool cetilestearílico	171215CSA/15272717	1
Caelo	Cetostearyl alcohol (type…	17132001	11
Caelo	Cetostearyl alcohol (type…	17139201	5
Caelo	Cetostearyl alcohol (type…	17198002	5
Caelo	Cetostearyl alcohol (type…	17198003	24
Caelo	Emulgade® 1000 NI	17210402	1
Caelo	Álcool cetílico	17234902	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Álcool cetílico	17234903	1
Caelo	Álcool cetílico	17234904	5
Caelo	Cetostearyl alcohol (type…	17261701	2
Caelo	Cetostearyl alcohol (type…	17261702	4
Caelo	Álcool cetilestearílico	17321303	9
Caelo	Álcool cetilestearílico	17321305	1
Caelo	Álcool cetilestearílico	17321319	1
Caelo	Álcool cetilestearílico	17321603	16
Caelo	Álcool cetílico	17321612	6
Caelo	Álcool cetilestearílico	17D28-B06-334609	1
Caelo	Cetostearyl alcohol (type…	17D28-B06-338141	2
Caelo	Cetostearyl alcohol (type…	17F21-B01-341021	1
Caelo	Cetostearyl alcohol (type…	18003401	1
Caelo	Cetostearyl alcohol (type…	18003404	13
Caelo	Cetostearyl alcohol (type…	18006205P-190719-1	1
Caelo	Cetostearyl alcohol (type…	18018001	4
Caelo	Cetostearyl alcohol (type…	18018002	1
Caelo	Cetostearyl alcohol (type…	18018003P-190308-2	1
Caelo	Cetostearyl alcohol (type…	18018005	9
Caelo	Cetostearyl alcohol (type…	18018006	2
Caelo	Cetostearyl alcohol (type…	18081201	1
Caelo	Álcool cetílico	18153102	17
Caelo	Álcool cetílico	18237701	19
Caelo	Álcool cetilestearílico	18248502	12
Caelo	Álcool cetilestearílico	18248510	3
Caelo	Cetostearyl alcohol (type…	18291403	2
Caelo	Cetostearyl alcohol (type…	18291404	16
Caelo	Cetostearyl alcohol (type…	18291406	4
Caelo	Cetostearyl alcohol (type…	18291407	10
Caelo	Cetostearyl alcohol (type…	18291408	1
Caelo	Álcool cetilestearílico	18A23-B04	1
Caelo	Cetostearyl alcohol (type…	18A23-B04-349155	1
Caelo	Álcool cetilestearílico	18A23-B04-352987	2
Caelo	Cetostearyl alcohol (type…	19005207P-191101-2	1
Caelo	Álcool cetílico	19012504	6
Caelo	Álcool cetílico	19012509	11
Caelo	Cetostearyl alcohol (type…	19032014B	1
Caelo	Cetostearyl alcohol (type…	19055206	5
Caelo	Cetostearyl alcohol (type…	191857002	23
Caelo	Cetostearyl alcohol (type…	19185702	24
Caelo	Cetostearyl alcohol (type…	19185703	3
Caelo	Álcool cetilestearílico	192139002	3
Caelo	Álcool cetilestearílico	192139007	3
Caelo	Emulgade® 1000 NI	192199001	2
Caelo	Álcool cetílico	192219005	16
Caelo	Cetostearyl alcohol (type…	192747003	9
Caelo	Cetostearyl alcohol (type…	192747007	27
Caelo	Álcool cetílico	192921001	9
Caelo	Álcool cetílico	200002637001	1
Caelo	Emulgade® 1000 NI	20000858003	3
Caelo	Emulgade® 1000 NI	20002050001	1
Caelo	Álcool cetílico	20002637001	18
Caelo	Álcool cetilestearílico	20002898002	5
Caelo	Álcool cetílico	20004011001	1
Caelo	Álcool cetílico	2002637001	1
Caelo	Cetostearyl alcohol (type…	2011404	1
Caelo	Álcool cetílico	20250112-1	1
Caelo	Cetostearyl alcohol (type…	20F30B01200749	1
Caelo	Cetostearyl alcohol (type…	210000566007	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Álcool cetilestearílico	21000059001	9
Caelo	Álcool cetilestearílico	21000059005	8
Caelo	Cetostearyl alcohol (type…	21000086001	23
Caelo	Cetostearyl alcohol (type…	21000086002	5
Caelo	Cetostearyl alcohol (type…	21000086003	1
Caelo	Álcool cetílico	210001593001	1
Caelo	Cetostearyl alcohol (type…	21000566	1
Caelo	Cetostearyl alcohol (type…	21000566005	1
Caelo	Cetostearyl alcohol (type…	21000566006	1
Caelo	Cetostearyl alcohol (type…	21000566007	13
Caelo	Álcool cetilestearílico	2100059001	1
Caelo	Cetostearyl alcohol (type…	2100086001	2
Caelo	Álcool cetilestearílico	21001071005	1
Caelo	Cetostearyl alcohol (type…	21001071007	5
Caelo	Álcool cetílico	21001593001	11
Caelo	Emulgade® 1000 NI	21002092002	2
Caelo	Emulgade® 1000 NI	21002092004	2
Caelo	Álcool cetílico	21002870003	5
Caelo	Cetostearyl alcohol (type…	21003223003	9
Caelo	Cetostearyl alcohol (type…	21003223008	5
Caelo	Cetostearyl alcohol (type…	21003223010	2
Caelo	Álcool cetilestearílico	21003928003	3
Caelo	Álcool cetilestearílico	22001324007	3
Caelo	Cetostearyl alcohol (type…	22001329004	2
Caelo	Álcool cetilestearílico	2201324007	1
Caelo	Cetostearyl alcohol (type…	23051503	1
Caelo	Cetostearyl alcohol (type…	23091402	1
Caelo	Cetostearyl alcohol (type…	24101305	1
Caelo	Cetostearyl alcohol (type…	25/AKD1	1
Caelo	Cetostearyl alcohol (type…	25051201	1
Caelo	Álcool cetílico	28101701	1
Caelo	Cetostearyl alcohol (type…	29091803	1
Caelo	Cetostearyl alcohol (type…	303935	1
Caelo	Cetostearyl alcohol (type…	31032015B	1
Caelo	Cetostearyl alcohol (type…	3256	1
Caelo	Cetostearyl alcohol (type…	5011505	1
Caelo	Cetostearyl alcohol (type…	608/10072017	1
Caelo	Álcool cetílico	7071807	1
Caelo	Álcool cetilestearílico	8041708	1
Caelo	Cetostearyl alcohol (type…	9170717	1
Caelo	Cetostearyl alcohol (type…	Unbekannt	1
Caeolo	Cetostearyl alcohol (type…	17056807	1
Caesar & Lorenz GmbH	Cetostearyl alcohol (type…	18291404	1
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	21003223003	1
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	18018005	1
Caesar & Loretz GmbH…	Álcool cetílico	22000377002	1
Caesar & Loretz GmbH…	Álcool cetilestearílico	11302101	1
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	192747005	1
Caesar & Loretz GmbH…	Álcool cetílico	21001593001	2
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	191857002	4
Caesar & Loretz GmbH…	Álcool cetílico	20002637001	1
Caesar & Loretz GmbH…	Álcool cetilestearílico	21000059001	1
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	21000086001	2
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	192747007	1
Caesar & Loretz GmbH…	Cetostearyl alcohol (type…	21000566007	1
Caesar & Loretz GmbH/Gehe	Cetostearyl alcohol (type…	18291401	1
Caesar & Loretz GmbH/Gehe	Álcool cetílico	20002637001	1
Caesar & Loretz GmbH/Gehe	Cetostearyl alcohol (type…	21000566006	1
Caesar & Loretz GmbH…	Álcool cetilestearílico	21001071007	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Álcool cetilestearílico	22001324007	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	18291404	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	191857002	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	21000086001	3
Caesar & Loretz GmbH...	Álcool cetilestearílico	19055206	1
Caesar & Loretz GmbH...	Álcool cetilestearílico	19185702	1
Caesar & Loretz GmbH...	Álcool cetilestearílico	21001071007	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	21003223008	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	21003223010	1
Caesar & Loretz GmbH...	Álcool cetílico	19012509	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	19185702	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	21000566007	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	21001071007	1
Caesar & Loretz GmbH/Sana	Álcool cetílico	192219005	2
Caesar & Loretz GmbH...	Álcool cetilestearílico	18291404	2
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	18291406	1
Caesar & Loretz GmbH...	Cetostearyl alcohol (type...	21000566007	1
Caesar & Loretz GmbH...	Álcool cetílico	21001593001	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	13233008	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	16119604	3
Caesar & Loretz GmbH	Álcool cetilestearílico	17056806	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	17132001	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	18018005	1
Caesar & Loretz GmbH	Emulgade® 1000 NI	18143802	1
Caesar & Loretz GmbH	Álcool cetílico	18153102	3
Caesar & Loretz GmbH	Álcool cetílico	18237701	3
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	18248502	5
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	18291403	2
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	18291404	2
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	18291407	1
Caesar & Loretz GmbH	Álcool cetílico	19012504	2
Caesar & Loretz GmbH	Álcool cetílico	19012509	2
Caesar & Loretz GmbH	Álcool cetilestearílico	19055206	3
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	191857002	5
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	19185702	6
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	19185704	1
Caesar & Loretz GmbH	Álcool cetilestearílico	192139002	3
Caesar & Loretz GmbH	Álcool cetilestearílico	192139007	3
Caesar & Loretz GmbH	Emulgade® 1000 NI	192199001	1
Caesar & Loretz GmbH	Álcool cetílico	192219005	4
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	192747005	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	192747007	9
Caesar & Loretz GmbH	Álcool cetilestearílico	192921001	3
Caesar & Loretz GmbH	Emulgade® 1000 NI	20000858003	1
Caesar & Loretz GmbH	Álcool cetílico	20001279002	1
Caesar & Loretz GmbH	Emulgade® 1000 NI	20002050001	2
Caesar & Loretz GmbH	Álcool cetílico	20002637001	7
Caesar & Loretz GmbH	Álcool cetilestearílico	20002898002	2
Caesar & Loretz GmbH	Álcool cetilestearílico	21000059001	3
Caesar & Loretz GmbH	Álcool cetílico	21000059005	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	21000086001	7
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	21000086003	2
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	21000566007	4
Caesar & Loretz GmbH	Álcool cetilestearílico	21001071007	1
Caesar & Loretz GmbH	Álcool cetílico	21001593001	2
Caesar & Loretz GmbH	Álcool cetílico	21002870003	2
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	21003223002	2
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	21003223003	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type...	21003223010	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Álcool cetilestearílico	21003928003	1
Caesar & Loretz GmbH	Álcool cetílico	22000377001	1
Caesar & Loretz GmbH	Álcool cetilestearílico	22001324007	1
Caesar & Loretz GmbH	Cetostearyl alcohol (type…	22001329004	3
Caesar & Loretz GmbH	Álcool cetilestearílico	22003074003	1
Caesar & Loretz/Gehe	Álcool cetílico	19012504	1
Caesar & Loretz/Geil…	Cetostearyl alcohol (type…	192747007	1
Caesar & Loretz	Cetostearyl alcohol (type…	18291407	1
Caesar & Noweda	Cetostearyl alcohol (type…	19185703	1
Caesar &Loretz GmbH	Cetostearyl alcohol (type…	12065703	1
Caesar&loretz,Phoenix	Cetostearyl alcohol (type…	14158201	1
Caesar&Loretz/Noweda	Cetostearyl alcohol (type…	15271405	1
Caesar/Lorenz	Cetostearyl alcohol (type…	13233005	1
Caesar/Noweda	Cetostearyl alcohol (type…	11343405	1
Caesar/Noweda	Cetostearyl alcohol (type…	12065707	1
Caesar/Noweda	Álcool cetilestearílico	15272705	1
Caesar/Noweda	Álcool cetilestearílico	2911E-01077	2
Calo/AHD	Álcool cetílico	192921001	1
Cealo/AHD	Álcool cetilestearílico	16106307	1
Cealo/Alliance Healthcare	Álcool cetilestearílico	18291403	1
Cealo/Sanacorp	Álcool cetilestearílico	21003223003	1
Cealo	Álcool cetilestearílico	15385602	2
Cealo	Álcool cetilestearílico	19012504	1
Celo/Jenne	Cetostearyl alcohol (type…	21000086001	1
Ebert-Jacobi	Álcool cetilestearílico	16230603	1
EuRho Anzag ek:3,47EUR	Álcool cetílico	110505501	1
EuRho	Álcool cetílico	1206020-01	1
Euro OTC	Cetostearyl alcohol (type…	10836573	1
Euro OTC	Álcool cetílico	1105055-01	1
Euro OTC	Álcool cetilestearílico	1107035-01	1
Euro OTC	Álcool cetilestearílico	1204015-01	1
Euro OTC	Álcool cetílico	1206020-01	1
Euro OTC	Álcool cetílico	1211002-01	2
Euro OTC	Cetostearyl alcohol (type…	1212019-01	1
Euro OTC	Cetostearyl alcohol (type…	1305035-01	2
Euro OTC	Cetostearyl alcohol (type…	1404019-01	2
Euro OTC	Cetostearyl alcohol (type…	1404019-02	2
Euro OTC	Cetostearyl alcohol (type…	1404019-03	1
Euro OTC	Cetostearyl alcohol (type…	14G31-B03-297610	1
Euro OTC	Álcool cetilestearílico	150401001	1
Euro OTC	Cetostearyl alcohol (type…	1504010-01	3
Euro OTC	Cetostearyl alcohol (type…	150410-01	1
Euro OTC	Álcool cetílico	1508014-01	1
Euro OTC	Álcool cetílico	150818C	1
Euro OTC	Cetostearyl alcohol (type…	1510043-01	4
Euro OTC	Cetostearyl alcohol (type…	15271403	2
Euro OTC	Cetostearyl alcohol (type…	1604013-02	5
Euro OTC	Cetostearyl alcohol (type…	1701031-01	5
Euro OTC	Álcool cetilestearílico	17050001-01	1
Euro OTC	Cetostearyl alcohol (type…	1705001-01	11
Euro OTC	Cetostearyl alcohol (type…	171001-02	1
Euro OTC	Cetostearyl alcohol (type…	1711001-02	5
Euro OTC	Cetostearyl alcohol (type…	17110011-01	1
Euro OTC	Álcool cetílico	18153102	1
Euro OTC	Cetostearyl alcohol (type…	2002033-01	3
Euro OTC	Cetostearyl alcohol (type…	2012002-01	1
Euro OTC	Álcool cetilestearílico	2012002-02	1
Euro OTC	Álcool cetilestearílico	20270912-2	1
Euro OTC	Cetostearyl alcohol (type…	21897043	1
Euro OTC	Álcool cetilestearílico	2806	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Gehe	Cetostearyl alcohol (type…	150401-01	1
Euroh/Noweda	Cetostearyl alcohol (type…	1504010-01	1
Fagro	Cetostearyl alcohol (type…	5211Q-01078	1
Fagron	Álcool cetilestearílico	10F17-N02	1
Fagron	Cetostearyl alcohol (type…	11499002	1
Fagron	Álcool cetilestearílico	11E17-N13	1
Fagron	Álcool cetilestearílico	11f30-n11	1
Fagron	Cetostearyl alcohol (type…	11L22-N09	1
Fagron	Álcool cetilestearílico	12/17-N05	1
Fagron	Cetostearyl alcohol (type…	12602-N04	1
Fagron	Álcool cetílico	12A-02N12	1
Fagron	Cetostearyl alcohol (type…	12C30-N01	2
Fagron	Álcool cetilestearílico	12E30-N13	1
Fagron	Álcool cetilestearílico	12g02-n04	1
Fagron	Cetostearyl alcohol (type…	12G02N04	1
Fagron	Cetostearyl alcohol (type…	12G02-N04	12
Fagron	Álcool cetilestearílico	12J17-N05	2
Fagron	Álcool cetilestearílico	12J17-NO5	1
Fagron	Cetostearyl alcohol (type…	12J29-N04	4
Fagron	Álcool cetilestearílico	12K22-N03	3
Fagron	Cetostearyl alcohol (type…	12L19-N03	8
Fagron	Álcool cetilestearílico	13C13-N13	1
Fagron	Cetostearyl alcohol (type…	13F07-N05	9
Fagron	Cetostearyl alcohol (type…	13I06-N04	1
Fagron	Cetostearyl alcohol (type…	13L17-B05	2
Fagron	Cetostearyl alcohol (type…	13L17B05289805	1
Fagron	Cetostearyl alcohol (type…	13L17-B05-289805	7
Fagron	Cetostearyl alcohol (type…	13L17-B05-289806	5
Fagron	Cetostearyl alcohol (type…	13L17-B05-289807	1
Fagron	Cetostearyl alcohol (type…	13L17-B05-294999	4
Fagron	Álcool cetilestearílico	14346201	1
Fagron	Cetostearyl alcohol (type…	14G31-B03	1
Fagron	Cetostearyl alcohol (type…	14G31-B03-297610	2
Fagron	Álcool cetilestearílico	14G31-B03-297611	1
Fagron	Cetostearyl alcohol (type…	14G31-B03-305612	4
Fagron	Cetostearyl alcohol (type…	15789271	2
Fagron	Cetostearyl alcohol (type…	15C31-B00-307062	1
Fagron	Cetostearyl alcohol (type…	15C31-B99-307062	5
Fagron	Cetostearyl alcohol (type…	15D24-B02	2
Fagron	Cetostearyl alcohol (type…	15D24-B02-308261	5
Fagron	Cetostearyl alcohol (type…	15D24-B02-311993	9
Fagron	Cetostearyl alcohol (type…	16/13-B01-327355	2
Fagron	Cetostearyl alcohol (type…	16/13-B01-331290	1
Fagron	Cetostearyl alcohol (type…	16/13-Bo1-327864	1
Fagron	Cetostearyl alcohol (type…	161006CSA	1
Fagron	Cetostearyl alcohol (type…	16990201	1
Fagron	Cetostearyl alcohol (type…	16B23-B07	1
Fagron	Cetostearyl alcohol (type…	16B23-B07-318218	4
Fagron	Cetostearyl alcohol (type…	16B23-B07-320384	7
Fagron	Cetostearyl alcohol (type…	16B23-B07-323025	3
Fagron	Cetostearyl alcohol (type…	16I13-B01	2
Fagron	Cetostearyl alcohol (type…	16I13-B01_326511	1
Fagron	Cetostearyl alcohol (type…	17028-B06-334609	1
Fagron	Cetostearyl alcohol (type…	171216CAE/0016830715	1
Fagron	Álcool cetílico	17321612	1
Fagron	Cetostearyl alcohol (type…	17894959	1
Fagron	Cetostearyl alcohol (type…	17D21-B01-341021	1
Fagron	Cetostearyl alcohol (type…	17D28-B06	2
Fagron	Cetostearyl alcohol (type…	17D28-B06-334609	6
Fagron	Cetostearyl alcohol (type…	17D28-B06-338141	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Álcool cetilestearílico	17F21-B01	1
Fagron	Cetostearyl alcohol (type…	17F21-B01-341021	10
Fagron	Cetostearyl alcohol (type…	17F21-B01-344775	3
Fagron	Cetostearyl alcohol (type…	18003401	1
Fagron	Cetostearyl alcohol (type…	18A12-B04-355659	1
Fagron	Álcool cetilestearílico	18A23-B04	1
Fagron	Cetostearyl alcohol (type…	18A23-B04-349155	8
Fagron	Cetostearyl alcohol (type…	18A23-B04-352987	6
Fagron	Cetostearyl alcohol (type…	18A23-B04-355659	2
Fagron	Álcool cetilestearílico	18A23-B64	1
Fagron	Cetostearyl alcohol (type…	19/04-B04-195303	1
Fagron	Cetostearyl alcohol (type…	19104-B04-195303	2
Fagron	Cetostearyl alcohol (type…	19I04-B04	1
Fagron	Cetostearyl alcohol (type…	19I04-B04-195303	5
Fagron	Álcool cetilestearílico	19I04-B04-195303	1
Fagron	Cetostearyl alcohol (type…	19II4-B04-195303	2
Fagron	Álcool cetilestearílico	19104-B04-195303	1
Fagron	Cetostearyl alcohol (type…	20260712-2	1
Fagron	Cetostearyl alcohol (type…	20F30B01200749	1
Fagron	Cetostearyl alcohol (type…	20F30-B01-200749	8
Fagron	Cetostearyl alcohol (type…	21139741	1
Fagron	Cetostearyl alcohol (type…	21J20-B05-213671	3
Fagron	Cetostearyl alcohol (type…	2215I-01078	1
Fagron	Cetostearyl alcohol (type…	22803390	1
Fagron	Cetostearyl alcohol (type…	22C11-B02-222108	1
Fagron	Cetostearyl alcohol (type…	2717M-01078	1
Fagron	Cetostearyl alcohol (type…	2797	1
Fagron	Cetostearyl alcohol (type…	2918E-01078	1
Fagron	Cetostearyl alcohol (type…	297611	1
Fagron	Cetostearyl alcohol (type…	3013M-01078	1
Fagron	Álcool cetilestearílico	3414E-01078	1
Fagron	Cetostearyl alcohol (type…	68955-20-4	1
Fagron	Álcool cetilestearílico	7886542	1
Fagron	Cetostearyl alcohol (type…	8256792	4
Fagron	Cetostearyl alcohol (type…	9652865	2
Fagron	Cetostearyl alcohol (type…	B04-1953003	1
fargon	Cetostearyl alcohol (type…	18A23-B04-352987	1
Fiebig	Álcool cetilestearílico	21000059001	1
Finze	Álcool cetílico	10321703	1
fragron	Cetostearyl alcohol (type…	16113-b01-326511	1
Gatt-Koller	Álcool cetílico	1690/06162416	1
Gatt-Koller	Álcool cetilestearílico	1803965	1
Gehe	Cetostearyl alcohol (type…	12L19-N03	1
Gehe	Álcool cetilestearílico	15272713	1
Gehe	Álcool cetilestearílico	15272717	1
Gehe	Cetostearyl alcohol (type…	1701031-01	1
Gehe	Álcool cetílico	18237701	1
Gehe	Cetostearyl alcohol (type…	18291406	1
Gehe	Álcool cetílico	19012504	1
Gehe	Cetostearyl alcohol (type…	22001329004	1
GEHE	Cetostearyl alcohol (type…	22001329908	1
Gehe	Cetostearyl alcohol (type…	22004149004	1
Gehe	Cetostearyl alcohol (type…	22004189	1
Gepepharm/Gehe	Álcool cetílico	181531102	1
Henry Lamotte / Noweda	Cetostearyl alcohol (type…	300132	1
Herba	Álcool cetilestearílico	KNC1133J18	1
Kehr	Álcool cetílico	17047303	1
Kehr	Cetostearyl alcohol (type…	18003404	1
Kehr	Cetostearyl alcohol (type…	22001329004	2
Klenk	Cetostearyl alcohol (type…	16238607	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Krieger	Cetostearyl alcohol (type…	1711001-01	1
Krieger	Álcool cetílico	19012509	1
L12	Cetostearyl alcohol (type…	17056806	1
Nachprüfung	Cetostearyl alcohol (type…	123456	2
Noweda/ Caesar&Loren…	Álcool cetílico	192921001	1
Noweda	Álcool cetilestearílico	12065709	1
Noweda	Cetostearyl alcohol (type…	13065576	1
Noweda	Cetostearyl alcohol (type…	13144104	1
Noweda	Cetostearyl alcohol (type…	13CA9	1
Noweda	Álcool cetilestearílico	17321303	1
Noweda	Cetostearyl alcohol (type…	18003404	1
Noweda	Cetostearyl alcohol (type…	18018005	1
Noweda	Álcool cetilestearílico	18248510	1
Noweda	Cetostearyl alcohol (type…	192747007	1
Noweda	Cetostearyl alcohol (type…	22001329008	2
Pala	Cetostearyl alcohol (type…	19185702	1
Ph.Eur/AHD	Álcool cetilestearílico	18291407	1
Phoenix 10.01.2020	Álcool cetílico	19012509	1
Phoenix 26.11.12	Cetostearyl alcohol (type…	13144105	1
PHOENIX am07.04.2014	Cetostearyl alcohol (type…	13F07-N05	1
Phoenix	Álcool cetilestearílico	14322505	1
Phoenix	Cetostearyl alcohol (type…	15789271	1
Phoenix	Cetostearyl alcohol (type…	17198003	1
Phoenix	Cetostearyl alcohol (type…	17D28-B06-338141	1
Phoenix	Emulgade® 1000 NI	18335402	1
Phoenix	Álcool cetilestearílico	18A23-B04-352987	1
Phoenix	Álcool cetilestearílico	192139007	1
Phoenix	Cetostearyl alcohol (type…	21003223010	1
Phoenix	Álcool cetilestearílico	3071	1
Phönix, Caesar&Loret…	Cetostearyl alcohol (type…	192747007	1
Phönix	Álcool cetílico	13096901	1
Phonix	Álcool cetílico	13210504	1
Phönix	Cetostearyl alcohol (type…	1323305	1
Phönix	Cetostearyl alcohol (type…	15C31-B99-307062	1
Phönix	Álcool cetilestearílico	17D28-B06-338141	1
Phönix	Cetostearyl alcohol (type…	18A23-B04-355659	1
Phönix	Cetostearyl alcohol (type…	191857002	1
Phönix	Cetostearyl alcohol (type…	19185702	1
Phönix	Cetostearyl alcohol (type…	20005694	1
Phönix	Cetostearyl alcohol (type…	21000566007	3
Phönix	Cetostearyl alcohol (type…	22001329008	1
Phönx	Cetostearyl alcohol (type…	210086001	1
Sanacorp/Bombstus	Cetostearyl alcohol (type…	18003437	2
Sanacorp	Cetostearyl alcohol (type…	12J29-N04	1
Sanacorp	Álcool cetilestearílico	13206206	1
Sanacorp	Cetostearyl alcohol (type…	13F07-N05	4
Sanacorp	Cetostearyl alcohol (type…	13I06-N04	1
Sanacorp	Cetostearyl alcohol (type…	15090701	1
Sanacorp	Cetostearyl alcohol (type…	17198003	1
Sanacorp	Álcool cetílico	17321603	1
Sanacorp	Cetostearyl alcohol (type…	191857002	1
Sanacorp	Cetostearyl alcohol (type…	210032230058	1
Sanacorp	Cetostearyl alcohol (type…	21003223011	2
Sanacorp	Emulgade® 1000 NI	22002953003	2
Sanacorp	Álcool cetilestearílico	22003074003	1
Sanacorp	Álcool cetilestearílico	575778	1
Sanacorpaelo /Sanacorp	Álcool cetílico	1AKS11	1
Spinnrad/ Noweda/ 19…	Álcool cetílico	219302021	1
Spinnrad/Sanacorp	Álcool cetílico	1018202022	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spinnrad	Álcool cetílico	115202022	1
Spinnrad	Álcool cetílico	416202023	1
Spinnrad	Álcool cetílico	418302021	1
spinrad/pHÖNIX	Álcool cetílico	418202021	1
Taoasis	Cetostearyl alcohol (type…	303935	2

- 234 468 spectra from 1515 *Apo-Ident* customers from a total of 48 862 batches from a further 718 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Álcool cetoestearílico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Álcool cetoestearílico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	2065	0	150 897
Type B	0	1260	0	200 824
Type C	0	1595	4	234 468

The substance/substance group *Álcool cetoestearílico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.7094 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5238 %)
Type C	100.0000 % (> 99.9007 %)	99.7498 % (> 99.5622 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20738	21054	7,42	80,12
20896	20896	0,00	128,52
20968	20968	0,00	132,51
21054	21054	0,00	75,39
21279	21279	0,00	135,00
21314	26698	21,65	128,73
21318	20896	50,16	127,68
21319	21319	0,00	125,14
21381	21998	17,95	86,62
21434	22334	3,89	134,97
21435	20896	49,97	126,88
21442	26698	14,63	130,04
21830	21998	3,37	102,21
21998	21998	0,00	114,65
22264	22334	3,46	135,55
22266	22266	0,00	129,51
22331	22331	0,00	129,37
22332	22332	0,00	143,48
22333	22333	0,00	122,59
22334	22334	0,00	135,13
22390	21054	9,70	88,16
22398	22398	0,00	129,71
22399	22399	0,00	129,43
22400	22400	0,00	128,89
22401	22401	0,00	128,69
22402	22402	0,00	128,23
22403	22403	0,00	132,29
22611	22401	27,08	123,94
23022	22334	3,45	136,84
23725	26698	15,07	131,87
25253	25253	0,00	93,08
25498	26695	11,76	133,67
25499	21998	27,05	130,21
25519	21054	10,12	88,11
25528	25528	0,00	132,26
25978	25978	0,00	35,03
26025	22333	8,99	109,37
26231	26698	11,90	132,18
26586	26695	6,51	132,49
26695	26695	0,00	132,11
26697	26697	0,00	129,39
26698	26698	0,00	133,19
26744	21054	10,75	89,18
26941	26941	0,00	132,52

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Álcool emulsificante não iônico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20467-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Álcool emulsificante não iônico; Alcoholes emulsificantes nonionici

Special notes

When selecting the *Álcool emulsificante não iônico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Álcool emulsificante não iônico	9	3	25

Second-stage model

For differentiation of the substance/substance group *Álcool emulsificante não iônico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Álcool emulsificante não iônico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cetostearyl alcohol (type A), emuls…	22,60	–
Emulgade® 1000 NI	31,30	–
Monoestearato de glicerol, emulsionante	43,93	–
Álcool cetilestearílico	47,80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Álcool emulsificante não iônico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Álcool emulsificante não iônico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	Álcool emulsificante não …	NS-8350010216	23274	40	20160718
apomix	Álcool emulsificante não …	NS-8350010618	24695	40	20180925
apomix	Álcool emulsificante não …	NS-8350010419	25391	40	20190527
apomix	Álcool emulsificante não …	NS-8350010720	26585	40	20220722
apomix	Álcool emulsificante não …	NS-8350010720	26585SI	20	20220722
Bombastus	Álcool emulsificante não …	19001210	24644	40	20190221
Bombastus	Álcool emulsificante não …	19001210	24664	40	20190221
Caelo	Álcool emulsificante não …	13413001	21069	40	1405257
Caelo	Álcool emulsificante não …	13413001	21524	40	20140116
Caelo	Álcool emulsificante não …	182021	24282	40	20180725*
Caelo	Álcool emulsificante não …	20002375001	25511	40	20200731
Caelo	Álcool emulsificante não …	21001521	25695	50	20210518*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 470 spectra of 12 reference samples from the substance/substance group *Álcool emulsificante não iônico*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 492 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Álcool emulsificante não iônico*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Álcool emulsificante não …	162231	22745	40
Caelo	Álcool emulsificante não …	171836	23576	40
Caelo	Álcool emulsificante não …	22003308004	26735	40
apomix	Álcool emulsificante não …	NS-8350010720	25864	50
apomix	Álcool emulsificante não …	NS-8350010720	25864SI	10
Caelo	Álcool emulsificante não …	22003308004	26735SI	20

- 201 884 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 68 spectra from 30 *Apo-Ident* customers from 28 batches from the substance/substance group *Álcool emulsificante não iônico*.

- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Álcool emulsificante não …	22003308002	1
	Álcool emulsificante não …	NS-8350010720	1
Bombastus	Álcool emulsificante não …	18005087P-190119-2	1
Bombastus	Álcool emulsificante não …	18005087P-190315-2	1
Bombastus	Álcool emulsificante não …	19001210	2
Bombastus	Álcool emulsificante não …	267575	2
Bombastus	Álcool emulsificante não …	274059	1
Bombastus	Álcool emulsificante não …	278281	4
Bombastus	Álcool emulsificante não …	284009	2
Bombastus	Álcool emulsificante não …	292319	8
Bombastus	Álcool emulsificante não …	295568	6
Bombastus	Álcool emulsificante não …	2995568	1
Bombastus	Álcool emulsificante não …	304997	5
Bombastus	Álcool emulsificante não …	3066	1
Bombastus	Álcool emulsificante não …	306665	1
Bombastus	Álcool emulsificante não …	306666	8
Bombastus	Álcool emulsificante não …	311625	2
Caelo	Álcool emulsificante não …	12254402	1
Caelo	Álcool emulsificante não …	14241503	1
Caelo	Álcool emulsificante não …	15287902	3
Caelo	Álcool emulsificante não …	18202102	1
Caelo	Álcool emulsificante não …	19045201	1
Caelo	Álcool emulsificante não …	20002375001	4
Caelo	Álcool emulsificante não …	20002375003	2
Caelo	Álcool emulsificante não …	2002375001	1
Caelo	Álcool emulsificante não …	21091302	1
Caelo	Álcool emulsificante não …	311625	1
Caesar & Loretz GmbH	Álcool emulsificante não …	18202102	1
E Plus	Álcool emulsificante não …	17043701	1
L11	Álcool emulsificante não …	17043701	1
L31	Álcool emulsificante não …	16223104	1
Phönix	Álcool emulsificante não …	274059	1

- 235 999 spectra from 1515 *Apo-Ident* customers from a total of 49 231 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Álcool emulsificante não iônico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Álcool emulsificante não iônico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	470	0	152 492
Type B	0	200	0	201 884
Type C	0	68	0	235 999

The substance/substance group *Álcool emulsificante não iônico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7234 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.1765 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21069	21069	0,00	45,61
21524	25695	10,70	37,52
23274	24282	13,35	46,09
24282	24282	0,00	53,77
24644	24282	12,16	47,47
24664	24282	12,26	51,95
24695	25695	7,41	44,40
25391	21069	17,98	31,30
25511	24282	26,95	59,42
25695	25695	0,00	53,88
26585	25695	17,02	37,66

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Alfaestradiol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20292-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Alfaestradiol; Alfatradiolum

Special notes

When selecting the *Alfaestradiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Alfaestradiol	10	18	262

Second-stage model

For differentiation of the substance/substance group *Alfaestradiol* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Alfaestradiol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	82,13	–
⋮	⋮	⋮
Capsaicina	>50	58,00
Levocarnitina	>50	120,77
Prednicarbato	>50	136,43
Citrato de sódio	>50	139,94
Cloridrato de oxibutinina	>50	152,64
Piridoxal-5-fosfato	>50	203,70
Acetato de noretisterona	>50	208,68
Tetracaína	>50	217,64
Acetato de ciproterona	>50	261,51
Cloridrato de amitriptilina	>50	449,51
Cloridrato de quinina di-hidratado	>50	470,77
Metoxisaleno	>50	574,96
Heparina sódica	>50	604,20
Valina	>50	650,36
Cloridrato de ciprofloxacina	>50	771,14
Amifampridina	>50	1497,50
Triclosan	>50	1598,25
Sacarose	>50	1997,63

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Alfaestradiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Alfaestradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Alfaestradiol	AP33-16-I-62P2985A	22935	40	20161017
Audor Pharma	Alfaestradiol	AP33-18-I-68P3620A	24662	40	20180804

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Alfaestradiol	13201601	21476	120	20130812
Caelo	Alfaestradiol	13201601	21477	60	20130812
Caelo	Alfaestradiol	191599	24747	40	20190812*
Caelo	Alfaestradiol	20004170	25553	40	20210106*
Caelo	Alfaestradiol	20004170	25553SI	40	20210106*
Caelo	Alfaestradiol	20002390	25561	40	20200914*
Caelo	Alfaestradiol	20002390	25561SI	40	20200914*
Euro OTC	Alfaestradiol	1404001-01	21714	50	1509288
Euro OTC	Alfaestradiol	1404001-01	21714SI	60	1509288
Euro OTC	Alfaestradiol	1603019	22511	40	20160419*
Euro OTC	Alfaestradiol	1603019	22511SI	40	20160419*
Fagron	Alfaestradiol	13G19-N06	20940	40	1402683
Fagron	Alfaestradiol	15J27-B08-323877	22933	40	20151117
Fagron	Alfaestradiol	15J27-B08-323877	22934	40	20151117
Fagron	Alfaestradiol	15J27-B08-323877	22934SI	40	20151117

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 810 spectra of 17 reference samples from the substance/substance group *Alfaestradiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 152 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1654 spectra of 41 reference samples from the substance/substance group *Alfaestradiol*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Alfaestradiol	161804	23354	40
Caelo	Alfaestradiol	191598	24738	40
Caelo	Alfaestradiol	22000052006	26740	40
Euro OTC	Alfaestradiol	1902020	24621	40
Euro OTC	Alfaestradiol	2002017	25118	40
Euro OTC	Alfaestradiol	2006005	25473	40
Euro OTC	Alfaestradiol	2103003	25689	50
Euro OTC	Alfaestradiol	2201003	25948	40
Euro OTC	Alfaestradiol	2301040	26601	40
Euro OTC	Alfaestradiol	2305010	26755	40
Euro OTC	Alfaestradiol	2305011	26756	30
Euro OTC	Alfaestradiol	2305012	26757	30
Euro OTC	Alfaestradiol	2305013	26758	40
Euro OTC	Alfaestradiol	2305014	26759	40
Euro OTC	Alfaestradiol	2310012	26998	40
Euro OTC	Alfaestradiol	2409001	27388	40
Euro OTC	Alfaestradiol	2409008	27389	40
Fagron	Alfaestradiol	22I06-B02-222372	26390	40
Audor Pharma	Alfaestradiol	AP33-16-I-62P2985A	22935SI†	40
Audor Pharma	Alfaestradiol	AP33-18-I-68P3620A	24662SI†	40
Caelo	Alfaestradiol	13201601	21477SI†	60
Caelo	Alfaestradiol	161804	23354SI	40
Caelo	Alfaestradiol	191598	24738SI	40
Caelo	Alfaestradiol	191599	24747SI†	40
Caelo	Alfaestradiol	22000052006	26740SI	40
Euro OTC	Alfaestradiol	1902020	24621SI	40
Euro OTC	Alfaestradiol	2002017	25118SI	40
Euro OTC	Alfaestradiol	2006005	25473SI	40
Euro OTC	Alfaestradiol	2103003	25689SI	50
Euro OTC	Alfaestradiol	2201003	25948SI	40
Euro OTC	Alfaestradiol	2301040	26601SI	40
Euro OTC	Alfaestradiol	2305010	26755SI	40
Euro OTC	Alfaestradiol	2305011	26756SI	40
Euro OTC	Alfaestradiol	2305012	26757SI	40
Euro OTC	Alfaestradiol	2305013	26758SI	34
Euro OTC	Alfaestradiol	2305014	26759SI	40
Euro OTC	Alfaestradiol	2310012	26998SI	40
Euro OTC	Alfaestradiol	2409001	27388SI	40
Euro OTC	Alfaestradiol	2409008	27389SI	40
Fagron	Alfaestradiol	15J27-B08-323877	22933SI†	40
Fagron	Alfaestradiol	22I06-B02-222372	26390SI	40

- 200 430 spectra from a total of 4022 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 955 spectra from 446 *Apo-Ident* customers from 271 batches from the substance/substance group *Alfaestradiol*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- Among them are spectra of independent samples from 262 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Alfaestradiol	2103003-01	1
	Alfaestradiol	21D20-F06-379262	1
	Alfaestradiol	21D20-F06-379263	1
	Alfaestradiol	22000052001	2
	Alfaestradiol	22000052002	1
	Alfaestradiol	2200052001	1
	Alfaestradiol	22A10-F02-381369	2
	Alfaestradiol	22I06-B02-222371	1
	Alfaestradiol	23000344003	1
	Alfaestradiol	23000344004	2
	Alfaestradiol	23000346002	4
	Alfaestradiol	2301040-01	1
	Alfaestradiol	24J10-B13-003480	1
	Alfaestradiol	f02-3813609	1
Alliance	Alfaestradiol	19159803	1
Anzag / Gehe	Alfaestradiol	14C20-B02-294943	1
Audor Pharma	Alfaestradiol	1617M-03305	1
Audor Pharma	Alfaestradiol	18C23-B05-352725	1
Audor Pharma	Alfaestradiol	2019Q-03305	1
Audor Pharma	Alfaestradiol	2818A-03305	1
Audor Pharma	Alfaestradiol	33-16-I-62P2985A	1
Audor Pharma	Alfaestradiol	33-18-I-68P3620A	1
Audor Pharma	Alfaestradiol	AP1404001-01A	1
Audor Pharma	Alfaestradiol	AP1404001-01-A	1
Audor Pharma	Alfaestradiol	AP1504015-01A	6
Audor Pharma	Alfaestradiol	AP21-16-II-14P4511	2
Audor Pharma	Alfaestradiol	AP21-16II-14P4511A	1
Audor Pharma	Alfaestradiol	AP21-16-II-14P4511A	9
Audor Pharma	Alfaestradiol	ap2116ll14p4511a	1
Audor Pharma	Alfaestradiol	AP33_16_I_62P2985A	1
Audor Pharma	Alfaestradiol	AP3316I42P2945A	1
Audor Pharma	Alfaestradiol	AP33-16-I-42P2945A	4
Audor Pharma	Alfaestradiol	AP3316I62P2985A	1
Audor Pharma	Alfaestradiol	AP33-16-I-62P2985A	4
Audor Pharma	Alfaestradiol	AP33-18-I68P3620A	1
Audor Pharma	Alfaestradiol	AP33-18-I-68P3620A	6
Audor Pharma	Alfaestradiol	AP35_17_II_85P3624A	1
Audor Pharma	Alfaestradiol	AP35-17-II-85P3524A	1
Audor Pharma	Alfaestradiol	AP35-17-II-85P3624	2
Audor Pharma	Alfaestradiol	AP35-17-II-85P3624-1A	2
Audor Pharma	Alfaestradiol	ap35-17-II-85P3624A	1
Audor Pharma	Alfaestradiol	AP35-17-II-85P3624A	4
Audor Pharma	Alfaestradiol	AP5100461A	2
Audor Pharma	Alfaestradiol	AP5104925A	6
Audor Pharma	Alfaestradiol	AP514925A	1
Audor Pharma	Alfaestradiol	APXP103DAA	2
Audor Pharma	Alfaestradiol	APXPC0071A	2
Bombastus	Alfaestradiol	16G05-B01-335789	1
cae	Alfaestradiol	20002390006	1
Caelo	Alfaestradiol	10319904	1
Caelo	Alfaestradiol	10319909	1
Caelo	Alfaestradiol	11061001	2
Caelo	Alfaestradiol	11061004	1
Caelo	Alfaestradiol	11061005	1
Caelo	Alfaestradiol	111161607	1
Caelo	Alfaestradiol	11161805	4
Caelo	Alfaestradiol	11161807	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alfaestradiol	12164201	4
Caelo	Alfaestradiol	12164207	7
Caelo	Alfaestradiol	12H29-N05	2
Caelo	Alfaestradiol	13130805	5
Caelo	Alfaestradiol	13130806	2
Caelo	Alfaestradiol	13130808	1
Caelo	Alfaestradiol	13201605	2
Caelo	Alfaestradiol	14037904	3
Caelo	Alfaestradiol	14130104	1
Caelo	Alfaestradiol	14139102	3
Caelo	Alfaestradiol	14139103	6
Caelo	Alfaestradiol	14139104	14
Caelo	Alfaestradiol	14139105	2
Caelo	Alfaestradiol	14318502	2
Caelo	Alfaestradiol	14318509	1
Caelo	Alfaestradiol	14318511	3
Caelo	Alfaestradiol	14318512	3
Caelo	Alfaestradiol	14318514	2
Caelo	Alfaestradiol	14C20-B02-294943	2
Caelo	Alfaestradiol	14C20-B02-294944	1
Caelo	Alfaestradiol	14I22-B30-302019	1
Caelo	Alfaestradiol	15356801	16
Caelo	Alfaestradiol	15356804	8
Caelo	Alfaestradiol	1536801	1
Caelo	Alfaestradiol	15380001	9
Caelo	Alfaestradiol	15G07-B01-310227	1
Caelo	Alfaestradiol	15G07-B01-311881	1
Caelo	Alfaestradiol	16087501	12
Caelo	Alfaestradiol	16087502	7
Caelo	Alfaestradiol	16087504	22
Caelo	Alfaestradiol	16087507	1
Caelo	Alfaestradiol	16087510	3
Caelo	Alfaestradiol	160875105728	1
Caelo	Alfaestradiol	16087511	2
Caelo	Alfaestradiol	16087512	9
Caelo	Alfaestradiol	16180406	4
Caelo	Alfaestradiol	16180408	7
Caelo	Alfaestradiol	16180409	19
Caelo	Alfaestradiol	16180412	1
Caelo	Alfaestradiol	16180413	2
Caelo	Alfaestradiol	16180415	2
Caelo	Alfaestradiol	16G05-B01-335789	1
Caelo	Alfaestradiol	16G05-B01-337353	1
Caelo	Alfaestradiol	16G-B01-328254	1
Caelo	Alfaestradiol	17G03-B11-341398	1
Caelo	Alfaestradiol	18180409	1
Caelo	Alfaestradiol	18C23-B05-354802	1
Caelo	Alfaestradiol	19159801	4
Caelo	Alfaestradiol	19159802	5
Caelo	Alfaestradiol	19159803	10
Caelo	Alfaestradiol	19159804	20
Caelo	Alfaestradiol	19159805	6
Caelo	Alfaestradiol	191599002	1
Caelo	Alfaestradiol	191599003	10
Caelo	Alfaestradiol	191599005	7
Caelo	Alfaestradiol	19A24-B03-360709	1
Caelo	Alfaestradiol	19K06-F04	1
Caelo	Alfaestradiol	20002390001	1
Caelo	Alfaestradiol	20002390003	11
Caelo	Alfaestradiol	20002390006	14

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alfaestradiol	20004170001	1
Caelo	Alfaestradiol	20004170003	2
Caelo	Alfaestradiol	20004170004	9
Caelo	Alfaestradiol	20004170006	6
Caelo	Alfaestradiol	20004170009	5
Caelo	Alfaestradiol	2000417001	1
Caelo	Alfaestradiol	2000417004	2
Caelo	Alfaestradiol	2061504	1
Caelo	Alfaestradiol	21D20-F06-378303	1
Caelo	Alfaestradiol	220000053005	2
Caelo	Alfaestradiol	22000052001	6
Caelo	Alfaestradiol	22000052002	8
Caelo	Alfaestradiol	22000053003	2
Caelo	Alfaestradiol	22000053004	4
Caelo	Alfaestradiol	22000053005	14
Caelo	Alfaestradiol	23000346006	1
Caelo	Alfaestradiol	2830	1
Caelo	Alfaestradiol	4318512	1
Caelo	Alfaestradiol	5051406	1
Caelo	Alfaestradiol	5107516	1
Caelo	Alfaestradiol	511211	1
Caeol/Noweda	Alfaestradiol	16180410	1
Caesar & Loretz GmbH...	Alfaestradiol	19159803	1
Caesar & Loretz GmbH...	Alfaestradiol	20002390004	1
Caesar & Loretz GmbH...	Alfaestradiol	20002390003	1
Caesar & Loretz GmbH/AEP	Alfaestradiol	20002390004	1
Caesar & Loretz GmbH/all	Alfaestradiol	191599003	1
Caesar & Loretz GmbH/GEHE	Alfaestradiol	20002390006	1
Caesar & Loretz GmbH/Gehe	Alfaestradiol	22000052002	1
Caesar & Loretz GmbH...	Alfaestradiol	20004170006	1
Caesar & Loretz GmbH/Kehr	Alfaestradiol	22000052002	1
Caesar & Loretz GmbH...	Alfaestradiol	19159804	1
Caesar & Loretz GmbH...	Alfaestradiol	20F18-F01-372920	2
Caesar & Loretz GmbH/P	Alfaestradiol	19159801	1
Caesar & Loretz GmbH...	Alfaestradiol	191599005	2
Caesar & Loretz GmbH/Sa	Alfaestradiol	19159803	1
Caesar & Loretz GmbH...	Alfaestradiol	19159805	1
Caesar & Loretz GmbH...	Alfaestradiol	20004170004	1
Caesar & Loretz GmbH...	Alfaestradiol	22000053005	1
Caesar & Loretz GmbH	Alfaestradiol	16087512	1
Caesar & Loretz GmbH	Alfaestradiol	16180407	1
Caesar & Loretz GmbH	Alfaestradiol	16180408	1
Caesar & Loretz GmbH	Alfaestradiol	16180409	1
Caesar & Loretz GmbH	Alfaestradiol	16180413	1
Caesar & Loretz GmbH	Alfaestradiol	19159801	2
Caesar & Loretz GmbH	Alfaestradiol	19159803	4
Caesar & Loretz GmbH	Alfaestradiol	19159804	2
Caesar & Loretz GmbH	Alfaestradiol	19159805	2
Caesar & Loretz GmbH	Alfaestradiol	191599002	1
Caesar & Loretz GmbH	Alfaestradiol	191599003	5
Caesar & Loretz GmbH	Alfaestradiol	191599005	5
Caesar & Loretz GmbH	Alfaestradiol	20002390003	3
Caesar & Loretz GmbH	Alfaestradiol	20002390004	1
Caesar & Loretz GmbH	Alfaestradiol	20002390006	3
Caesar & Loretz GmbH	Alfaestradiol	20004170001	2
Caesar & Loretz GmbH	Alfaestradiol	20004170004	5
Caesar & Loretz GmbH	Alfaestradiol	20004170006	5
Caesar & Loretz GmbH	Alfaestradiol	20004170009	3
Caesar & Loretz GmbH	Alfaestradiol	22000052002	4
Caesar & Loretz GmbH	Alfaestradiol	22000052003	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Alfaestradiol	22000053003	3
Caesar & Loretz GmbH	Alfaestradiol	22000053004	1
Caesar & Loretz GmbH	Alfaestradiol	22000053005	4
Caesar & Loretz GmbH	Alfaestradiol	AP33-18-I-68P3620A	1
Caesar & Loretz/Sanacorp	Alfaestradiol	16180409	1
Caesar und Loretz GmbH	Alfaestradiol	16087502	1
Caesar&Lorenz/Phoenix	Alfaestradiol	16087502	1
Caesar&Loretz GmbH/Anzag	Alfaestradiol	12164207	1
Caesar/Lorenz	Alfaestradiol	11061001	1
carlo	Alfaestradiol	10319903	1
Chiracon GmbH	Alfaestradiol	AP35-17-II-85P3624	1
Chiracon/Phoenix	Alfaestradiol	35-19-I-14P3693	1
Euro OTC	Alfaestradiol	121696	1
Euro OTC	Alfaestradiol	1404001-01	2
Euro OTC	Alfaestradiol	1404001-02	1
Euro OTC	Alfaestradiol	15356804	1
Euro OTC	Alfaestradiol	160301901	1
Euro OTC	Alfaestradiol	1603019-03	3
Euro OTC	Alfaestradiol	16087510	2
Euro OTC	Alfaestradiol	16180410	1
Euro OTC	Alfaestradiol	2002017-01	1
Euro OTC	Alfaestradiol	200201702	1
Euro OTC	Alfaestradiol	2002017-02	2
Euro OTC	Alfaestradiol	20060005-01	1
Euro OTC	Alfaestradiol	2006005-01	3
Euro OTC	Alfaestradiol	2103003-01	7
Euro OTC	Alfaestradiol	2201003-01	9
Euro OTC	Alfaestradiol	2201830-01	1
Euro OTC	Alfaestradiol	2209016-01	1
Euro OTC	Alfaestradiol	2301040-01	1
Euro OTC	Alfaestradiol	AP21-16-II-14P4511A	1
Euro OTC	Alfaestradiol	AP33-16-I-62P2985A	1
Euro OTC	Alfaestradiol	AP33-16-l-62P2985A	1
Fagron	Alfaestradiol		2
Fagron	Alfaestradiol	11B07-N05	1
Fagron	Alfaestradiol	11D07-N19	1
Fagron	Alfaestradiol	11G22-N11	2
Fagron	Alfaestradiol	11k25-N01	1
Fagron	Alfaestradiol	11K25-N01	3
Fagron	Alfaestradiol	12D19-N03	6
Fagron	Alfaestradiol	12H29-N05	4
Fagron	Alfaestradiol	12J27-B08-314546	1
Fagron	Alfaestradiol	12L19-N08	7
Fagron	Alfaestradiol	12L19-No8	1
Fagron	Alfaestradiol	13201605	1
Fagron	Alfaestradiol	1372918	1
Fagron	Alfaestradiol	13G19-N06	19
Fagron	Alfaestradiol	13G19-N06	1
Fagron	Alfaestradiol	13G19-N09	1
Fagron	Alfaestradiol	13G19-No6	2
Fagron	Alfaestradiol	13L30B32	1
Fagron	Alfaestradiol	13L30-B32	2
Fagron	Alfaestradiol	13L30-B32-290739	1
Fagron	Alfaestradiol	13L30B32-290741	1
Fagron	Alfaestradiol	13130b32290742	1
Fagron	Alfaestradiol	13L30-B32-290742	1
Fagron	Alfaestradiol	14/22-B30-302017	3
Fagron	Alfaestradiol	14722-B30-302018	1
Fagron	Alfaestradiol	14C20-B02-294943	4
Fagron	Alfaestradiol	14C20-B02-294944	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Alfaestradiol	14G07-B99	1
Fagron	Alfaestradiol	14G07-B99-294942	1
Fagron	Alfaestradiol	14G07-B99-294945	4
Fagron	Alfaestradiol	14I22-B30	1
Fagron	Alfaestradiol	15G07-B01	1
Fagron	Alfaestradiol	15G07-B01-310227	5
Fagron	Alfaestradiol	15G07-B01-310228	3
Fagron	Alfaestradiol	15G07-B01-310229	3
Fagron	Alfaestradiol	15G07-B01-311881	2
Fagron	Alfaestradiol	15J27-B08	1
Fagron	Alfaestradiol	15J27-B08-314546	1
Fagron	Alfaestradiol	15J27B08318164	1
Fagron	Alfaestradiol	15J27-B08-318164	3
Fagron	Alfaestradiol	15J27-B08-318783	1
Fagron	Alfaestradiol	15J27-B08-321786	2
Fagron	Alfaestradiol	16G05-801	1
Fagron	Alfaestradiol	16g05-b01-324614	1
Fagron	Alfaestradiol	16G05-B01-324614	1
Fagron	Alfaestradiol	16G05-B01-325108	1
Fagron	Alfaestradiol	16G05-B01-326866	1
Fagron	Alfaestradiol	16G05-B01-328254	1
Fagron	Alfaestradiol	16G05-B01-332379	4
Fagron	Alfaestradiol	16G05-B01-334055	3
Fagron	Alfaestradiol	16G05-B01-335789	7
Fagron	Alfaestradiol	16G05-B01-337352	3
Fagron	Alfaestradiol	16G05-B01-337353	1
Fagron	Alfaestradiol	16G05-Bo1-332379	1
Fagron	Alfaestradiol	16G05-N01-335789	1
Fagron	Alfaestradiol	17G03-B11	4
Fagron	Alfaestradiol	17G03-B11_348862	1
Fagron	Alfaestradiol	17G03-B11-341398	2
Fagron	Alfaestradiol	17G03-B11-341399	2
Fagron	Alfaestradiol	17G03-B11-345093	5
Fagron	Alfaestradiol	17G03-B11-346962	1
Fagron	Alfaestradiol	17G03-B11-348862	2
Fagron	Alfaestradiol	17G03-B11-348863	1
Fagron	Alfaestradiol	18C23-B05	2
Fagron	Alfaestradiol	18C23-B05_350996	1
Fagron	Alfaestradiol	18C23-B05_354802	1
Fagron	Alfaestradiol	18C23-B05-350996	4
Fagron	Alfaestradiol	18C23-B05-352724	2
Fagron	Alfaestradiol	18C23-B05-352725	1
Fagron	Alfaestradiol	18C23-B05-354802	9
Fagron	Alfaestradiol	18C23-B05-356316	2
Fagron	Alfaestradiol	18C23-B05-4802	1
Fagron	Alfaestradiol	19A24-B003360712	1
Fagron	Alfaestradiol	19A24-B03	3
Fagron	Alfaestradiol	19A24-B03_360710	1
Fagron	Alfaestradiol	19A24-B03-360709	3
Fagron	Alfaestradiol	19A24-B03-360710	13
Fagron	Alfaestradiol	19AB03360709	1
Fagron	Alfaestradiol	19K06-F04	1
Fagron	Alfaestradiol	19K06F04366005	1
Fagron	Alfaestradiol	19K06-F04-366005	10
Fagron	Alfaestradiol	19K06-F04-366006	2
Fagron	Alfaestradiol	19K06-F04-366007	2
Fagron	Alfaestradiol	20122-F02-374255	2
Fagron	Alfaestradiol	20122-F02-374256	1
Fagron	Alfaestradiol	20F18-F01	1
Fagron	Alfaestradiol	20F18F01372918	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Alfaestradiol	20F18-F01-372918	15
Fagron	Alfaestradiol	20F18-F01372920	1
Fagron	Alfaestradiol	20F18-F01-372920	2
Fagron	Alfaestradiol	20F8-FD1	1
Fagron	Alfaestradiol	20I22-F02-374255	3
Fagron	Alfaestradiol	20I22-F02-374256	2
Fagron	Alfaestradiol	21D20_F06_379262	1
Fagron	Alfaestradiol	21D20-F036-379262	1
Fagron	Alfaestradiol	21D20-F06	2
Fagron	Alfaestradiol	21D20F06378303	2
Fagron	Alfaestradiol	21D20-F06-378303	6
Fagron	Alfaestradiol	21D20-F06-378305	2
Fagron	Alfaestradiol	21D20-F06-378306	2
Fagron	Alfaestradiol	21D20-F06-378476	3
Fagron	Alfaestradiol	21d20f06379262	1
Fagron	Alfaestradiol	21D20-F06-379262	10
Fagron	Alfaestradiol	21D20-F06-379263	2
Fagron	Alfaestradiol	22A10-F02-381369	7
Fagron	Alfaestradiol	22A10-F02-381421	1
Fagron	Alfaestradiol	23E15-B08-224470	1
Fagron	Alfaestradiol	2735	1
Fagron	Alfaestradiol	324614	1
Fagron	Alfaestradiol	5102432	1
Fagron	Alfaestradiol	5111184	2
Fagron	Alfaestradiol	5115018	1
Fagron	Alfaestradiol	5119507	4
Fagron	Alfaestradiol	5122243	6
Fagron	Alfaestradiol	5122244	1
Fagron	Alfaestradiol	6882484	1
Fagron	Alfaestradiol	9011904	1
Fagron	Alfaestradiol	F01-3729103	1
Fagron	Alfaestradiol	F04-3660005	1
Fagron	Alfaestradiol	F04-3660006	1
Fagron	Alfaestradiol	F0637926002	1
Fagron	Alfaestradiol	XP101UT	1
Fargon/AHD	Alfaestradiol	17G03-B11	1
Fargon/Kehr	Alfaestradiol	16G05-B01-332379	1
Fargon	Alfaestradiol	21D20-F06-379262	1
Fgron / Alliance Healthc.	Alfaestradiol	16G05-B01-328254	1
Fiebig/Farago	Alfaestradiol	19A24-B03-360709	1
fragon/phonix	Alfaestradiol	17G03-B11-341399	1
Gatt-Koller	Alfaestradiol	180077661	1
Gatt-Koller	Alfaestradiol	1803210	2
Gehe/Fragron	Alfaestradiol	5111184	2
Gehe	Alfaestradiol	16087501	1
GEHE	Alfaestradiol	16087512	1
Gehe	Alfaestradiol	19159801	1
Gehe	Alfaestradiol	22000053007	1
gepepharm/Phoenix	Alfaestradiol	19054203	2
Hirsch	Alfaestradiol	12L19-N08	2
Kehr	Alfaestradiol	18C23-B05-350996	1
Kehr	Alfaestradiol	19K06-F04-3660055	1
Kwizda	Alfaestradiol	529068	1
Noweda am 10.08.2018	Alfaestradiol	16087510	1
Noweda/Fragron	Alfaestradiol	16G05-B01-332379	1
Noweda	Alfaestradiol	16G05-B01-324614	2
Noweda	Alfaestradiol	19159803	1
Noweda	Alfaestradiol	21D20-F06-378303	1
Noweda	Alfaestradiol	22000053007	1
Noweda	Alfaestradiol	22A10-F02-381369	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Alfaestradiol	2301040-01	1
Phönix	Alfaestradiol	15356801	1
Phönix	Alfaestradiol	21D20-F06-378305	1
Phönix	Alfaestradiol	33-18-1-68P3620A	1
Phönix	Alfaestradiol	APXPC0071A	1
Phönix	Alfaestradiol	B05-3509906	1
Proquina / Gehe	Alfaestradiol	15356801	1
Proquina / Gehe	Alfaestradiol	19A24-B03-360711	1
Proquina / Gehe	Alfaestradiol	5122243	1
Proquina / Gehe	Alfaestradiol	6882478	1
Proquina / Gehe	Alfaestradiol	F04-3660006	1
Proquina / Sanacorp	Alfaestradiol	F04-3660005	1
Sanacorp, 39,57EUR, 27.1.17	Alfaestradiol	700670-0011	1
Sanacorp	Alfaestradiol	13201605	1
Sanacorp	Alfaestradiol	15356804	1
Sanacorp	Alfaestradiol	19159802	2
Sanacorp	Alfaestradiol	2103003-01	1
Sanacorp	Alfaestradiol	21D20-F06-379262	1
Sanacorp	Alfaestradiol	22A10-F02-381369	1
Shandong Northwest M...	Alfaestradiol	AEC160522	1
Shandong northwest m...	Alfaestradiol	AEC151211	1
VDL 1.7.14;40.30 euro	Alfaestradiol	13G19-N06	1

- 235 112 spectra from 1515 *Apo-Ident* customers from a total of 48 991 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Alfaestradiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Alfaestradiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	810	0	152 152
Type B	0	1654	0	200 430
Type C	0	941	14	235 112

The substance/substance group *Alfaestradiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2593 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6372 %)
Type C	100.0000 % (> 99.9007 %)	98.5340 % (> 98.2199 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20940	20940	0,00	115,46
21476	22511	22,09	125,52
21477	22511	24,74	124,97
21714	21714	0,00	122,09
22511	22511	0,00	119,66
22933	22511	9,60	120,08
22934	22511	5,03	119,49
22935	25553	9,42	131,49
24662	24747	40,23	128,00
24747	24747	0,00	128,70
25553	25553	0,00	130,55
25561	25561	0,00	129,02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Alopurinol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22243-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Alopurinol; Allopurinolum

Special notes

When selecting the *Alopurinol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Alopurinol	4	2	17

Second-stage model

For differentiation of the substance/substance group *Alopurinol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Alopurinol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	112,68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Alopurinol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Alopurinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Alopurinol	14E15-B05-307746	22243	60	AR-16-FG-004367-01
Fagron	Alopurinol	14E15-B05-315557	22345	60	20140611
Fagron	Alopurinol	14E15-B05-307746	22836	40	20140611
Fagron	Alopurinol	22H29-B06-223774	26450	40	20220930
Fagron	Alopurinol	23D12-B06-228657	26818	40	20230510

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Alopurinol*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 722 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Alopurinol*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Alopurinol	14E15-B05-330859	23523	40
Fagron	Alopurinol	18E23-B02-357777	24577	40
Fagron	Alopurinol	14E15-B05-330859	23526	40
Fagron	Alopurinol	22H29-B06-223774	26450SI†	20
Fagron	Alopurinol	23D12-B06-228657	26818SI†	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 19 *Apo-Ident* customers from 19 batches from the substance/substance group *Alopurinol*.
- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Alopurinol	14E15-B05-337862	4
Caesar & Loretz GmbH	Alopurinol	18E23-B02-350905	1
Fagron	Alopurinol	14E15-B05_315557	1
Fagron	Alopurinol	14E15-B05-315557	14
Fagron	Alopurinol	14E15B05-320787	1
Fagron	Alopurinol	14E15-B05-320787	1
Fagron	Alopurinol	14E15-B08	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Alopurinol	18E23-B02	1
Fagron	Alopurinol	18E23-B02-350905	1
Fagron	Alopurinol	18E23-B02-357777	3
Fagron	Alopurinol	18E23-B02-361600	1
Fagron	Alopurinol	190261502	1
Fagron	Alopurinol	19061206	1
Fagron	Alopurinol	200250306	1
Fagron	Alopurinol	200803107	1
Fagron	Alopurinol	22H29-B06-223774	1
Fagron	Alopurinol	B02-3509005	1
Fagron	Alopurinol	B02-3577707	1
Fagron	Alopurinol	B02-3616000	1
Phönix	Alopurinol	200612506	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Alopurinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Alopurinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	160	0	201 924
Type C	0	38	0	236 029

The substance/substance group *Alopurinol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.2105 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22243	22243	0,00	190,96
22345	22243	3,54	193,07
22836	22243	4,08	194,26
26450	22243	8,29	194,35
26818	22243	15,00	194,55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amido**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20790-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amido; Amido de arroz; Amido de milho; Amido de trigo; Amylum Maydis; Amylum oryzae; Fécula de batata; Solani amylum; SyrSpend® SF Alka; SyrSpend® SF pH4; SyrSpend® SF pH4 neo; Tritici amylum

Special notes

When selecting the *Amido* substance/substance group, the following information is displayed to the user:

- Nota sobre identificação do SyrSpend® SF Alka: Agite a amostra antes da medição para garantir a distribuição uniforme das partículas.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Amido	39	28	521

Second-stage model

For differentiation of the substance/substance group *Amido* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Amido* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Maltodextrina	27,19	21,32
Goma arábica, dispersão seca	32,16	19,94
Cromoglicato de sódio	49,44	–
Sulfato de polimixina B	74,98	31,26
⋮	⋮	⋮
Carmelose sódica	>50	15,48
Sulfato de colistina	>50	27,30
Glicerofosfato de cálcio	>50	34,10
Cianocobalamina	>50	42,15
Anfotericina B	>50	42,30
Bacitracina	>50	48,19
Riboflavina	>50	58,24
Levedura de selênio	>50	61,71
Tosilcloramida sódica	>50	70,62
Ácido oxálico	>50	74,74
Frutose	>50	75,79
Pantotenato de cálcio	>50	77,29
Nistatina	>50	78,88
Gelatina, branca	>50	95,04
Bromidrato de hioscina	>50	103,52
Vitamina E acetato pó 50%	>50	117,17
Estradiol hemi-hidratado	>50	124,00
Triancinolona	>50	130,27
Metilcobalamina	>50	153,73
Estriol	>50	165,95

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Amido* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Amido*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Amido de arroz	12068525	20790	40	20120327
Caelo	Amido de arroz	16144501	22585	40	20160504
Euro OTC	Amido de arroz	1912005	25080	40	20200109*
Euro OTC	Amido de arroz	2101008	25534	40	20210129*
Euro OTC	Amido de arroz	2107016	25767	50	20210816*
Fagron	Amido de arroz	16B25-B01-327231	23219	40	20160308
Fagron	Amido de arroz	16B25-B01-327231	23220	40	AR-17-FG-015298-02
Caelo	Amido de milho	13154914	21827	60	20130529
Caelo	Amido de milho	161385	22450	60	20160621*
Caelo	Amido de milho	182748	24361	40	20181031*
Caelo	Amido de milho	24001513	27324	40	20240722*
Klenk	Amido de milho	0064A200427-01	25383	40	20200515
Caelo	Amido de trigo	14023203	21447	60	AR-16-FG-011433-01
Caelo	Amido de trigo	15124707	22246	60	20150527
Caelo	Amido de trigo	23002728	27107	40	20240123*
Klenk	Amido de trigo	0104A141114	21973	60	20141210
Klenk	Amido de trigo	0104A160512	23510	40	20160628
Caelo	Fécula de batata	12360213	20996	40	1403494
Caelo	Fécula de batata	14033815	21965	60	20140207
Caelo	Fécula de batata	161237	22449	60	20160621*
Caelo	Fécula de batata	24001388	27321	40	20240722*
Klenk	Fécula de batata	0094A170123	23923	40	20170309
Klenk	Fécula de batata	0094A180919-01	25382	40	20200804
Fagron	SyrSpend® SF Alka	17D11-B04-332593	23448	40	20170505
Fagron	SyrSpend® SF Alka	17D11-B04-332593	23449	40	20170505
Fagron	SyrSpend® SF Alka	17F14-B02-335945	23750	20	1804106
Fagron	SyrSpend® SF Alka	18B21-B08-347192	24112	40	1809264
Fagron	SyrSpend® SF Alka	18C13-B11-350851	24290	40	20180502
Fagron	SyrSpend® SF Alka	20B25-F06-369913	25363	40	20200424
Fagron	SyrSpend® SF Alka	23B16-F01-384773	27029	40	20230502
Fagron	SyrSpend® SF pH4	15A26-B04-311720	22496	40	1608352
Fagron	SyrSpend® SF pH4	15A26-B04-311720	22497	40	20150223
Fagron	SyrSpend® SF pH4	15A26-B04-305667	22719	40	1701055
Fagron	SyrSpend® SF pH4	19L05-F10-368874	25369	40	20200320
Fagron	SyrSpend® SF pH4	22L20-F03-384076	26613	40	20230124
Fagron	SyrSpend® SF pH4	22L20-F03-384076	26613SI	20	20230124
Fagron	SyrSpend® SF pH4	23H11-F02-385247	27030	40	20231005
Fagron	SyrSpend® SF pH4	23E23-F05-385178	27056	40	20230807
Fagron	SyrSpend® SF pH4 neo	21G23-F02-379002	25755	50	2112411
Fagron	SyrSpend® SF pH4 neo	23A18-H15-00941	26568	40	20230120
Fagron	SyrSpend® SF pH4 neo	23C21-H01-00941	26677	40	20230328
Fagron	SyrSpend® SF pH4 neo	23C21-H01-00941	26677SI	20	20230328
Fagron	SyrSpend® SF pH4 neo	23K02-H08-00941	27180	40	20231113
Fagron	SyrSpend® SF pH4 neo	24B28-H08-00941	27192	40	20240308

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1860 spectra of 44 reference samples from the substance/substance group *Amido*. These samples are listed above in the *calibration samples* section. The reference samples come from 39 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 151 102 spectra from a total of 2803 batches from further 479 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1550 spectra of 47 reference samples from the substance/substance group *Amido*.
- Among them are spectra of independent samples from 28 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Amido de arroz	162180	22642	40
Caelo	Amido de arroz	190169	24551	40
Caelo	Amido de arroz	190168	24553	40
Caelo	Amido de arroz	20001724	25661	40
Caelo	Amido de arroz	23001380	27254	40
Caelo	Amido de arroz	2405002	27276	40
Euro OTC	Amido de arroz	2204008	26200	40
Euro OTC	Amido de arroz	2301042	26596	40
Euro OTC	Amido de arroz	2309004	26932	40
Caelo	Amido de milho	16138505	23217	40
Caelo	Amido de milho	172873	23813	40
Caelo	Amido de milho	170474	24037	40
Caelo	Amido de trigo	15421507	23509	40
Caelo	Amido de trigo	181200	24014	40
Caelo	Amido de trigo	192516	24885	40
Caelo	Fécula de batata	15062921	23189	40
Caelo	Fécula de batata	173003	23811	40
Caelo	Fécula de batata	20001764	25660	40
Caelo	Fécula de batata	21004156	26015	30
Fagron	SyrSpend® SF Alka	15H11-B04-311722	22494	40
Fagron	SyrSpend® SF Alka	22B04-F07-381936	26457	40
Fagron	SyrSpend® SF Alka	22K18-F04-38394	27028	40
Fagron	SyrSpend® SF pH4	15H13-B03-314611	23450	40
Fagron	SyrSpend® SF pH4	16J10-B03-330757	23749	40
Fagron	SyrSpend® SF pH4	23B13-F02-384539	26731	40
Fagron	SyrSpend® SF pH4 neo	22B04-F01-381138	25936	40
Fagron	SyrSpend® SF pH4 neo	23L01-H01-00941	27181	40
Fagron	SyrSpend® SF pH4 neo	24A09-H07-00941	27182	40
Euro OTC	Amido de arroz	2204008	26200SI	20
Euro OTC	Amido de arroz	2301042	26596SI	20
Euro OTC	Amido de arroz	2309004	26932SI	20
Caelo	Amido de milho	24001513	27324SI†	20
Caelo	Amido de trigo	23002728	27107SI†	20
Caelo	Fécula de batata	21004156	26015SI	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fécula de batata	24001388	27321SI†	20
Fagron	SyrSpend® SF Alka	15H11-B04-311722	22495	40
Fagron	SyrSpend® SF Alka	15H11-B04-311722	22718	40
Fagron	SyrSpend® SF Alka	17F14-B02-335945	23750†	20
Fagron	SyrSpend® SF Alka	15H11-B04-311722	23768	40
Fagron	SyrSpend® SF Alka	22B04-F07-381936	26457SI	20
Fagron	SyrSpend® SF Alka	22K18-F04-38394	27028SI	20
Fagron	SyrSpend® SF Alka	23B16-F01-384773	27029SI†	20
Fagron	SyrSpend® SF pH4	15H13-B03-314611	23451	40
Fagron	SyrSpend® SF pH4	23B13-F02-384539	26731SI	20
Fagron	SyrSpend® SF pH4	23H11-F02-385247	27030SI†	20
Fagron	SyrSpend® SF pH4 neo	22B04-F01-381138	25936SI	10
Fagron	SyrSpend® SF pH4 neo	23K02-H08-00941	27180SI†	20

- 200 534 spectra from a total of 4010 batches from further 836 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1837 spectra from 490 *Apo-Ident* customers from 538 batches from the substance/substance group *Amido*.
- Among them are spectra of independent samples from 502 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amido de trigo	104A221027-01	2
	Amido de milho	20004426022	1
	Amido de arroz	20004428022	3
	Amido de arroz	20004428041	1
	Amido de trigo	21002057002	1
	SyrSpend® SF pH4	22109-F01-283384	1
	SyrSpend® SF Alka	22A12-F20-381408	1
	SyrSpend® SF Alka	22A12-F22-382195	4
	SyrSpend® SF Alka	22B04-F06-381564	1
	SyrSpend® SF Alka	22B04-F07-381936	2
	SyrSpend® SF pH4	22I09-F02-383489	1
	SyrSpend® SF pH4	22I09-F03	1
	SyrSpend® SF pH4	22I09-F03-383490	2
	SyrSpend® SF Alka	22J04F02383639	1
	SyrSpend® SF Alka	22J04-F02-383639	2
	SyrSpend® SF Alka	22J04-F06-3636502	3
	SyrSpend® SF Alka	22J04-F06-383652	8
	SyrSpend® SF Alka	22J04-F08-383658	4
	SyrSpend® SF Alka	22J04-F11-383746	5
	SyrSpend® SF Alka	22J31-F01-526993	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	SyrSpend® SF Alka	22j31-F01-526993	1
	SyrSpend® SF Alka	22J04-F06-383652	1
	SyrSpend® SF pH4	22K08-F02-383826	6
	SyrSpend® SF pH4	22k08-F02-93826	1
	SyrSpend® SF Alka	22K17-F04-384631	1
	SyrSpend® SF Alka	22K17-F05-384376	1
	SyrSpend® SF Alka	22K18-F01-384185	1
	SyrSpend® SF pH4	22L20-F03-384076	2
	Amido de arroz	23001380003	2
	SyrSpend® SF pH4	23A03-F09-384187	1
	SyrSpend® SF pH4	23A03-F10-384538	1
	SyrSpend® SF Alka	23A18-F07-384725	3
	SyrSpend® SF pH4	23B13-F02-384539	2
	SyrSpend® SF pH4	23B13-F02-3845309	1
	SyrSpend® SF Alka	23B16-F01-384773	3
	SyrSpend® SF Alka	23B16-F02-384774	2
	SyrSpend® SF Alka	23B16-F03-384777	2
	SyrSpend® SF pH4	23E22-F03-384948	1
	SyrSpend® SF pH4	23E23-F05-385116	1
	Amido de milho	30502-01	2
	Amido de arroz	84A180522	1
	SyrSpend® SF Alka	F01-3847703	1
	SyrSpend® SF pH4	F02-2845309	1
	SyrSpend® SF Alka	F0238363009	1
	SyrSpend® SF pH4	F05-3811006	1
	SyrSpend® SF Alka	F07-3819306	1
	SyrSpend® SF pH4 neo	H09-0094001	1
AHD	SyrSpend® SF Alka	22J04-F06-383652	2
AHD	SyrSpend® SF Alka	22K17-F05-384376	1
AHD	SyrSpend® SF Alka	23A18-F07-384725	1
AHD	Amido de milho	64A170123	1
AHD	Amido de milho	64A230502-01	1
Alliance Healthcare	SyrSpend® SF Alka	20G03-F12-374282	1
Alliance	Amido de trigo	192516005	1
Anzag 05.03.13 ek: 9,65EUR	Amido de trigo	104A120621	2
Anzag	SyrSpend® SF pH4	23E22-F01-384947	1
Bombastus	Fécula de batata	12214303	2
Bombastus	Amido de milho	15310902	1
Bombastus	SyrSpend® SF pH4	18I16-B01-357703	1
Caelo	Amido de arroz	10061134	2
Caelo	Amido de milho	10061146	1
Caelo	Amido de arroz	10177507	1
Caelo	Amido de arroz	10177515	1
Caelo	Amido de arroz	104A120621	1
Caelo	Amido de arroz	104A141114	3
Caelo	Amido de trigo	104A160512	1
Caelo	Amido de trigo	104A171122	1
Caelo	Amido de arroz	11132406	1
Caelo	Amido de trigo	11145011	1
Caelo	Amido de trigo	11146011	1
Caelo	Amido de trigo	1114611	1
Caelo	Amido de milho	11179307	2
Caelo	Amido de arroz	11186026	1
Caelo	Fécula de batata	11301012	2
Caelo	Amido de trigo	11350907	1
Caelo	Amido de trigo	11350911	2
Caelo	Amido de arroz	12166007	3
Caelo	Amido de arroz	12214303	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Amido de milho	12238705	1
Caelo	Amido de arroz	12238714	1
Caelo	Amido de milho	12238715	2
Caelo	Amido de arroz	12238719	1
Caelo	SyrSpend® SF Alka	12B23-B07-305668	1
Caelo	Amido de arroz	13005905	2
Caelo	Amido de arroz	13005908	1
Caelo	Amido de arroz	13154904	3
Caelo	Amido de arroz	13154914	2
Caelo	Amido de arroz	13305103	3
Caelo	Amido de arroz	13305108	1
Caelo	Amido de arroz	14011612	3
Caelo	Amido de arroz	14011621	1
Caelo	Amido de arroz	14011630	2
Caelo	Amido de arroz	14023203	3
Caelo	Amido de arroz	14025710	1
Caelo	Amido de arroz	14025733	1
Caelo	Amido de arroz	14025734	1
Caelo	Fécula de batata	14033815	1
Caelo	Amido de milho	14111701	1
Caelo	Amido de arroz	14301214	3
Caelo	Fécula de batata	15062912	2
Caelo	Fécula de batata	15062915	1
Caelo	Amido de arroz	15118607	1
Caelo	Amido de arroz	15119011	6
Caelo	Amido de trigo	15124707	2
Caelo	Amido de trigo	15124710	1
Caelo	Amido de trigo	1512477	1
Caelo	Amido de milho	15210908	2
Caelo	Amido de milho	15310902	5
Caelo	Amido de milho	15310903	3
Caelo	Amido de milho	15310904	1
Caelo	Amido de milho	15310908	3
Caelo	Amido de milho	15310909	2
Caelo	Amido de milho	15310914	6
Caelo	Amido de trigo	15421507	2
Caelo	Amido de arroz	16101401	1
Caelo	Amido de milho	16138505	5
Caelo	Amido de milho	16138507	4
Caelo	Amido de arroz	16144506	1
Caelo	Amido de trigo	16162905	3
Caelo	Amido de arroz	16218002	2
Caelo	Amido de arroz	16218009	1
Caelo	Amido de arroz	16218013	1
Caelo	SyrSpend® SF pH4	16J10-B03-330757	1
Caelo	Fécula de batata	17037404	1
Caelo	Amido de milho	17047404	12
Caelo	Amido de arroz	17173501	2
Caelo	Amido de trigo	17183201	1
Caelo	Amido de milho	17287302	7
Caelo	Amido de milho	17287305	2
Caelo	Amido de milho	17287306	1
Caelo	Fécula de batata	17327201	3
Caelo	Amido de arroz	17327502	1
Caelo	Amido de arroz	17327503	2
Caelo	Amido de arroz	17327506	2
Caelo	Amido de milho	17327601	2
Caelo	Amido de trigo	18120004	2
Caelo	Amido de trigo	18120012	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	SyrSpend® SF Alka	18125-B15-357803	1
Caelo	Fécula de batata	182059005	2
Caelo	Fécula de batata	18205905	3
Caelo	Amido de milho	18274802	9
Caelo	Amido de milho	18274804	11
Caelo	Amido de milho	18274808	2
Caelo	SyrSpend® SF Alka	18871B06	1
Caelo	SyrSpend® SF pH4	18A22_B05_346147	1
Caelo	SyrSpend® SF Alka	18B21-B08	1
Caelo	SyrSpend® SF Alka	18C13-B11-350851	1
Caelo	SyrSpend® SF Alka	18H01-B12-353473	1
Caelo	SyrSpend® SF pH4	18H30-B02	1
Caelo	SyrSpend® SF Alka	18J25-B15-357803	2
Caelo	Amido de arroz	190168001	1
Caelo	Amido de arroz	190168003	5
Caelo	Amido de arroz	190168004	3
Caelo	Amido de arroz	19016801	1
Caelo	Amido de arroz	19016803	8
Caelo	Amido de arroz	19016805	1
Caelo	Amido de milho	1918702	1
Caelo	Amido de milho	191878005	3
Caelo	Amido de milho	19187802	7
Caelo	Amido de milho	19187803	1
Caelo	Amido de trigo	192516001	2
Caelo	Amido de trigo	192516005	4
Caelo	Amido de milho	20000573002	6
Caelo	Fécula de batata	20003937003	1
Caelo	Amido de milho	20004426002	1
Caelo	Amido de milho	20004426005	5
Caelo	Amido de milho	20004426010	1
Caelo	Amido de milho	20004426013	1
Caelo	Amido de milho	2000442602	1
Caelo	Amido de arroz	20004428002	2
Caelo	Amido de arroz	20004428003	1
Caelo	Amido de arroz	20004428022	1
Caelo	Amido de arroz	200613K3	1
Caelo	SyrSpend® SF pH4	20A09-F03-369540	1
Caelo	Amido de trigo	21002057001	3
Caelo	Amido de trigo	21002057006	1
Caelo	Amido de trigo	21002057007	1
Caelo	Amido de arroz	2212M-01115	1
Caelo	Amido de arroz	23001380004	1
Caelo	SyrSpend® SF Alka	353473	1
Caelo	Amido de arroz	64A130304	6
Caelo	Amido de milho	64A170123	1
Caelo	Amido de milho	64A200427-01	1
Caelo	SyrSpend® SF Alka	720026-000	1
Caelo	Amido de arroz	9352108	1
Caelo	Fécula de batata	94A18091901	1
Caesar & Loretz GmbH/AHD	Amido de milho	20000573002	1
Caesar & Loretz GmbH...	Amido de trigo	192516001	1
Caesar & Loretz GmbH/Gehe	Amido de milho	18274808	1
Caesar & Loretz GmbH/Gehe	Amido de milho	19187802	2
Caesar & Loretz GmbH/Sana	Amido de trigo	21002057001	1
Caesar & Loretz GmbH	Amido de trigo	16162908	2
Caesar & Loretz GmbH	Amido de arroz	17327510	1
Caesar & Loretz GmbH	Amido de trigo	18120012	1
Caesar & Loretz GmbH	Amido de milho	18274802	1
Caesar & Loretz GmbH	Amido de milho	18274804	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Amido de arroz	190168004	5
Caesar & Loretz GmbH	Amido de trigo	192516005	1
Caesar & Loretz GmbH	Amido de milho	20000573002	2
Caesar & Loretz GmbH	Amido de milho	20004426006	2
Caesar & Loretz GmbH	Amido de trigo	21000570005	1
Caesar & Loretz GmbH	Amido de trigo	21002057001	1
Caesar & Loretz/Geil...	Amido de milho	19187802	1
Cealo/Sanacorp	Amido de milho	17287302	1
Cealo/Sanacorp	Amido de milho	20000573002	1
Cealo	Amido de arroz	13305103	1
Cealo	Amido de trigo	15421507	1
Euro OTC	Amido de trigo	104A171122	1
Euro OTC	SyrSpend® SF pH4	18A22-B05-347899	1
Euro OTC	SyrSpend® SF pH4	20F18-F13-379343	1
Euro OTC	Amido de milho	64A170123	1
Fagon/Novatis	SyrSpend® SF pH4	20F08-f03	1
Fagron	SyrSpend® SF Alka		2
Fagron	SyrSpend® SF pH4	11111346	1
Fagron	Amido de arroz	12L19-N06	1
Fagron	Amido de milho	14011627	1
Fagron	Amido de arroz	14F18-B04-301616	1
Fagron	SyrSpend® SF Alka	14I22-B40-311723	1
Fagron	SyrSpend® SF Alka	14J22-B40-311723	2
Fagron	Amido de milho	15310902	1
Fagron	SyrSpend® SF pH4	15A26-B04-305667	1
Fagron	SyrSpend® SF Alka	15K03-B01-525173	1
Fagron	SyrSpend® SF pH4	16/10-B03	1
Fagron	SyrSpend® SF pH4	16710-B03	1
Fagron	SyrSpend® SF Alka	16B03-B07-525234	1
Fagron	SyrSpend® SF pH4	16J10_B03_330757	1
Fagron	SyrSpend® SF pH4	16J10B03	1
Fagron	SyrSpend® SF pH4	16J10-B03	3
Fagron	SyrSpend® SF pH4	16j10-b03-330757	1
Fagron	SyrSpend® SF pH4	16J10B03330757	1
Fagron	SyrSpend® SF pH4	16J10-B03-330757	8
Fagron	Amido de milho	17287302	1
Fagron	SyrSpend® SF Alka	17D11-804-332593	1
Fagron	SyrSpend® SF Alka	17D11-B04	2
Fagron	SyrSpend® SF Alka	17D11-B04-332593	7
Fagron	SyrSpend® SF Alka	17D11-bo4-332593	1
Fagron	SyrSpend® SF Alka	17D29-B11	1
Fagron	SyrSpend® SF Alka	17F14802-335945	1
Fagron	SyrSpend® SF Alka	17F14B02-335945	1
Fagron	SyrSpend® SF Alka	17F14-B02-335945	5
Fagron	SyrSpend® SF Alka	17F14-B05	1
Fagron	SyrSpend® SF Alka	17F14-B05-525556	2
Fagron	SyrSpend® SF pH4	18/16-B01-357703	1
Fagron	SyrSpend® SF Alka	18/25-B15-357803	1
Fagron	SyrSpend® SF Alka	18125-B15-357803	1
Fagron	SyrSpend® SF Alka	181C13-B11-350851	1
Fagron	SyrSpend® SF Alka	18821-808-147192	1
Fagron	SyrSpend® SF Alka	18821-b08-347192	1
Fagron	SyrSpend® SF Alka	18821-B08-347192	5
Fagron	SyrSpend® SF pH4	18A22_B04_346147	1
Fagron	SyrSpend® SF pH4	18A22-B05	2
Fagron	SyrSpend® SF pH4	18A22-B05-346147	6
Fagron	SyrSpend® SF pH4	18A22-B05-347899	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	18A26-B05	1
Fagron	SyrSpend® SF Alka	18a26b05346410	1
Fagron	SyrSpend® SF Alka	18A26-B05-346410	4
Fagron	SyrSpend® SF Alka	18A26-Bo5-346410	1
Fagron	SyrSpend® SF Alka	18B21-B08	2
Fagron	SyrSpend® SF Alka	18B21-B08-347192	3
Fagron	SyrSpend® SF Alka	18C13_B11_350851	1
Fagron	SyrSpend® SF Alka	18C13-B11	5
Fagron	SyrSpend® SF Alka	18C13-B11-350851	8
Fagron	SyrSpend® SF Alka	18C-B11-350851	1
Fagron	SyrSpend® SF Alka	18H01-812353473	1
Fagron	SyrSpend® SF Alka	18H01-b12	1
Fagron	SyrSpend® SF Alka	18H01-B12	7
Fagron	SyrSpend® SF Alka	18h01b12353473	1
Fagron	SyrSpend® SF Alka	18H01-B12353473	1
Fagron	SyrSpend® SF Alka	18H01-B12-353473	24
Fagron	SyrSpend® SF Alka	18H13-B12-353473	1
Fagron	SyrSpend® SF pH4	18H30_B02_355226	2
Fagron	SyrSpend® SF pH4	18H30-355226	1
Fagron	SyrSpend® SF pH4	18H30-B02	8
Fagron	SyrSpend® SF pH4	18H30B02355226	1
Fagron	SyrSpend® SF pH4	18H30-B02-355226	9
Fagron	SyrSpend® SF Alka	18I25-B15-357803	1
Fagron	SyrSpend® SF pH4	18J16_B01_357703	1
Fagron	SyrSpend® SF pH4	18J16-B01	2
Fagron	SyrSpend® SF pH4	18J16B01357703	1
Fagron	SyrSpend® SF pH4	18J16-B01-357703	12
Fagron	SyrSpend® SF Alka	18J21B113659901	1
Fagron	SyrSpend® SF Alka	18j25-B15	1
Fagron	SyrSpend® SF Alka	18J25B15	1
Fagron	SyrSpend® SF Alka	18J25-B15	6
Fagron	SyrSpend® SF Alka	18j25b15357803	1
Fagron	SyrSpend® SF Alka	18J25-B15357803	1
Fagron	SyrSpend® SF Alka	18J25-B15-357803	21
Fagron	SyrSpend® SF Alka	18L21-B11	11
Fagron	SyrSpend® SF Alka	18l21-b11-359901	2
Fagron	SyrSpend® SF Alka	18L21B11359901	1
Fagron	SyrSpend® SF Alka	18L21-B11-359901	16
Fagron	SyrSpend® SF Alka	18L21-B113659901	1
Fagron	SyrSpend® SF Alka	18L25-B15-357803	1
Fagron	SyrSpend® SF pH4	19/10-F09-367004	1
Fagron	SyrSpend® SF Alka	19029-B07-362182	1
Fagron	SyrSpend® SF pH4	19A14-B07	3
Fagron	SyrSpend® SF pH4	19A14-B07_362431	1
Fagron	SyrSpend® SF pH4	19A14-B07-362431	5
Fagron	SyrSpend® SF Alka	19D29-807	1
Fagron	SyrSpend® SF Alka	19D29807362182	1
Fagron	SyrSpend® SF Alka	19D29B07	1
Fagron	SyrSpend® SF Alka	19D29-B07	1
Fagron	SyrSpend® SF Alka	19d29b07362182	1
Fagron	SyrSpend® SF Alka	19D29-B07-362182	18
Fagron	SyrSpend® SF Alka	19D29-B11-363786	5
Fagron	SyrSpend® SF Alka	19D29-Bo7-362182	1
Fagron	SyrSpend® SF Alka	19F06-B002	1
Fagron	SyrSpend® SF Alka	19F06-B02	7
Fagron	SyrSpend® SF Alka	19F06-B02_363789	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	19F06-b02-363789	2
Fagron	SyrSpend® SF Alka	19F06-B02-363789	29
Fagron	SyrSpend® SF Alka	19F12	1
Fagron	SyrSpend® SF Alka	19F12-804-364057	1
Fagron	SyrSpend® SF Alka	19F12-B04	6
Fagron	SyrSpend® SF Alka	19-F12-B04	1
Fagron	SyrSpend® SF Alka	19F12-B04-364057	13
Fagron	SyrSpend® SF Alka	19F12-B04-36-4057	1
Fagron	SyrSpend® SF Alka	19F12-B07	2
Fagron	SyrSpend® SF Alka	19F12-B07-526149	8
Fagron	SyrSpend® SF Alka	19F12-BO4-364057	3
Fagron	SyrSpend® SF pH4	19J10-F08	8
Fagron	SyrSpend® SF pH4	19J10-F08-3669903	1
Fagron	SyrSpend® SF pH4	19j10-F08-366992	1
Fagron	SyrSpend® SF pH4	19J10-F08-366992	2
Fagron	SyrSpend® SF pH4	19J10-f08366993	1
Fagron	SyrSpend® SF pH4	19J10-F08-366993	7
Fagron	SyrSpend® SF pH4	19j10F09	1
Fagron	SyrSpend® SF pH4	19J10-F09	5
Fagron	SyrSpend® SF pH4	19j10-f09-364007	1
Fagron	SyrSpend® SF pH4	19J10-F09-366992	1
Fagron	SyrSpend® SF pH4	19j10-f09-367004	2
Fagron	SyrSpend® SF pH4	19j10-F09-367004	1
Fagron	SyrSpend® SF pH4	19J10-F09-367004	6
Fagron	SyrSpend® SF pH4	19J10-FO8-366992	1
Fagron	SyrSpend® SF Alka	19K007-F04	1
Fagron	SyrSpend® SF Alka	19K07-F04	4
Fagron	SyrSpend® SF Alka	19K07F04367548	1
Fagron	SyrSpend® SF Alka	19K07-F04-367548	5
Fagron	SyrSpend® SF Alka	19k07fo4	1
Fagron	SyrSpend® SF Alka	19K07-FO4-367548	6
Fagron	SyrSpend® SF Alka	19Ko7-F04-367548	1
Fagron	SyrSpend® SF pH4	19L05-F10	5
Fagron	SyrSpend® SF pH4	19L05-F10-3688704	1
Fagron	SyrSpend® SF pH4	19L05-f10-368874	1
Fagron	SyrSpend® SF pH4	19L05-F10-368874	13
Fagron	SyrSpend® SF pH4	19L05-F1O-368874	1
Fagron	SyrSpend® SF pH4	19LO5-F10-368874	1
Fagron	SyrSpend® SF pH4	1BL21-B11	1
Fagron	SyrSpend® SF Alka	20817-F03	1
Fagron	SyrSpend® SF Alka	20818F03	1
Fagron	SyrSpend® SF Alka	20818-F03-369574	3
Fagron	SyrSpend® SF Alka	20825f0625F06	1
Fagron	SyrSpend® SF Alka	20825-F06-369913	3
Fagron	SyrSpend® SF Alka	20825-F07	1
Fagron	SyrSpend® SF Alka	20825-F07-3669914	2
Fagron	SyrSpend® SF Alka	20825-F07369914	2
Fagron	SyrSpend® SF Alka	20825-F07-369914	2
Fagron	SyrSpend® SF Alka	20825-O6-3669913	1
Fagron	SyrSpend® SF Alka	2085-F06	1
Fagron	SyrSpend® SF pH4	20A09-F03	11
Fagron	SyrSpend® SF pH4	20A09-F03-369540	7
Fagron	SyrSpend® SF pH4	20A09-F03-3695400	1
Fagron	SyrSpend® SF Alka	20B18-F03	3
Fagron	SyrSpend® SF Alka	20B18-F03-369574	10
Fagron	SyrSpend® SF Alka	20B25-F06	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	20B25-F06_369913	1
Fagron	SyrSpend® SF Alka	20B25-F06-369913	29
Fagron	SyrSpend® SF Alka	20B25-F07	8
Fagron	SyrSpend® SF Alka	20B25-F07-369914	9
Fagron	SyrSpend® SF Alka	20B25-F07-369914	1
Fagron	SyrSpend® SF Alka	20B818-F03-369574	2
Fagron	SyrSpend® SF pH4	20c24-F02	1
Fagron	SyrSpend® SF pH4	20C24-F02	8
Fagron	SyrSpend® SF pH4	20c24-f02-372398	1
Fagron	SyrSpend® SF pH4	20c24-F02-372398	1
Fagron	SyrSpend® SF pH4	20C24-F02-372398	17
Fagron	SyrSpend® SF pH4	20C24-F09	1
Fagron	SyrSpend® SF pH4	20C24-F02	2
Fagron	SyrSpend® SF Alka	20D15-F08	1
Fagron	SyrSpend® SF Alka	20D15-F08-371028	2
Fagron	SyrSpend® SF Alka	20D16-F01	1
Fagron	SyrSpend® SF Alka	20D16-F06	1
Fagron	SyrSpend® SF pH4	20F08_F03_372517	1
Fagron	SyrSpend® SF pH4	20F08-F03	5
Fagron	SyrSpend® SF pH4	20F08-F03-0000	1
Fagron	SyrSpend® SF pH4	20F08-F03-372517	19
Fagron	SyrSpend® SF pH4	20F08-F04-372518	1
Fagron	SyrSpend® SF pH4	20F18-F13-379343	22
Fagron	SyrSpend® SF pH4	20F18-F14	2
Fagron	SyrSpend® SF Alka	20F18-F14-379344	11
Fagron	SyrSpend® SF Alka	20G03-F09-526400	1
Fagron	SyrSpend® SF Alka	20G03-F11	3
Fagron	SyrSpend® SF Alka	20G03-F11-374279	20
Fagron	SyrSpend® SF Alka	20G03-F12	2
Fagron	SyrSpend® SF Alka	20G03-F12-374282	6
Fagron	SyrSpend® SF Alka	20Go3-f12-374282	1
Fagron	SyrSpend® SF Alka	21101_F-02	1
Fagron	SyrSpend® SF Alka	21101-F02	1
Fagron	SyrSpend® SF Alka	21101-F02-380031	4
Fagron	SyrSpend® SF pH4	211021-01	1
Fagron	SyrSpend® SF Alka	21826-F08	1
Fagron	SyrSpend® SF Alka	21826-F08-379141	2
Fagron	SyrSpend® SF Alka	21926-F07-378133	1
Fagron	SyrSpend® SF Alka	21A21-376829	3
Fagron	SyrSpend® SF Alka	21A21-F01	5
Fagron	SyrSpend® SF Alka	21A21-F01-376829	18
Fagron	SyrSpend® SF Alka	21A21-FO1	1
Fagron	SyrSpend® SF Alka	21B26-F06	2
Fagron	SyrSpend® SF Alka	21B26-F07-378133	9
Fagron	SyrSpend® SF Alka	21B26-F08	2
Fagron	SyrSpend® SF Alka	21B26-F08-379141	10
Fagron	SyrSpend® SF Alka	21B26-FO6	1
Fagron	SyrSpend® SF Alka	21B26-F07378133	1
Fagron	SyrSpend® SF Alka	21F08-F03	3
Fagron	SyrSpend® SF Alka	21F08F03378828	1
Fagron	SyrSpend® SF Alka	21F08-F03-378828	20
Fagron	SyrSpend® SF Alka	21F08-F04	1
Fagron	SyrSpend® SF Alka	21F08-F04-378832	5
Fagron	SyrSpend® SF Alka	21F24F01379228	1
Fagron	SyrSpend® SF Alka	21F24-F01-379228	17
Fagron	SyrSpend® SF Alka	21F24-F01-37928	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	21F24-F03-379228	1
Fagron	SyrSpend® SF Alka	21F24-F03526598	1
Fagron	SyrSpend® SF Alka	21F24-F03-526598	3
Fagron	SyrSpend® SF Alka	21F24-F04	2
Fagron	SyrSpend® SF Alka	21F24-F04-379672	4
Fagron	SyrSpend® SF Alka	21F24-F01	1
Fagron	SyrSpend® SF Alka	21F08-F03-378828	1
Fagron	SyrSpend® SF Alka	21H16-F06	1
Fagron	SyrSpend® SF Alka	21H16-F06-0000	1
Fagron	SyrSpend® SF Alka	21H16F06379894	1
Fagron	SyrSpend® SF Alka	21H16-F06-379894	27
Fagron	SyrSpend® SF Alka	21H16-F06	1
Fagron	SyrSpend® SF pH4	21H20-F02-380674	9
Fagron	SyrSpend® SF Alka	21I01-F02	1
Fagron	SyrSpend® SF Alka	21I01-F02-380031	28
Fagron	SyrSpend® SF pH4	21K22-F06	1
Fagron	SyrSpend® SF Alka	21l01-F02-380031	1
Fagron	SyrSpend® SF Alka	21L07-F04-381033	2
Fagron	SyrSpend® SF Alka	21L07-F05	5
Fagron	SyrSpend® SF Alka	21L07F05381032	1
Fagron	SyrSpend® SF Alka	21L07-F05-381032	42
Fagron	SyrSpend® SF Alka	21L-07-F05-381032	1
Fagron	SyrSpend® SF pH4	22007-F04	1
Fagron	SyrSpend® SF pH4	22109-F02	1
Fagron	SyrSpend® SF pH4	22109-F03-383490	1
Fagron	SyrSpend® SF Alka	22804-F06	1
Fagron	SyrSpend® SF Alka	22804-F06-381564	1
Fagron	SyrSpend® SF Alka	22A12F20381408	1
Fagron	SyrSpend® SF Alka	22A12-F20-381408	5
Fagron	SyrSpend® SF Alka	22A12-F21	1
Fagron	SyrSpend® SF Alka	22A12F21526828	1
Fagron	SyrSpend® SF Alka	22A12-F21-526828	3
Fagron	SyrSpend® SF Alka	22A12-F22-382195	11
Fagron	SyrSpend® SF Alka	22A12-F24-382104	5
Fagron	SyrSpend® SF Alka	22B04-F04-381555	2
Fagron	SyrSpend® SF Alka	22B04F05-3819009	1
Fagron	SyrSpend® SF Alka	22B04-F05-381909	2
Fagron	SyrSpend® SF Alka	22B04-F05-381975	1
Fagron	SyrSpend® SF Alka	22B04-F06	2
Fagron	SyrSpend® SF Alka	22B04F06-381564	1
Fagron	SyrSpend® SF Alka	22B04-F06-381564	12
Fagron	SyrSpend® SF Alka	22B04-F07-381936	2
Fagron	SyrSpend® SF pH4	22B04-F02381139	1
Fagron	SyrSpend® SF Alka	22B04-F06-381564	1
Fagron	SyrSpend® SF pH4	22C07-F03	2
Fagron	SyrSpend® SF pH4	22C07-F03-382305	6
Fagron	SyrSpend® SF pH4	22C07-F04	1
Fagron	SyrSpend® SF pH4	22C07-F04-0000	1
Fagron	SyrSpend® SF pH4	22C07F04382813	1
Fagron	SyrSpend® SF pH4	22C07-F04-382813	8
Fagron	SyrSpend® SF pH4	22G07-H08	1
Fagron	SyrSpend® SF pH4	22I09-F01-383384	3
Fagron	SyrSpend® SF pH4	22I09-F02-383489	8
Fagron	SyrSpend® SF Alka	22J04-F02-383639	7
Fagron	SyrSpend® SF Alka	22J04-F0-2383639	1
Fagron	SyrSpend® SF Alka	22J04-F06-383652	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	22J31-F01-526993	1
Fagron	SyrSpend® SF Alka	22J4-F06-383652	1
Fagron	SyrSpend® SF pH4	22J04-F06-383652	1
Fagron	SyrSpend® SF pH4	22K01-H01	1
Fagron	SyrSpend® SF pH4	22K08F02-383826	1
Fagron	SyrSpend® SF pH4	22K08-F02-383826	6
Fagron	SyrSpend® SF pH4	22109-F01-383384	1
Fagron	SyrSpend® SF pH4	22109-F03-383490	1
Fagron	SyrSpend® SF pH4	22L20-F03-384076	1
Fagron	SyrSpend® SF pH4	23A03-F10-384538	1
Fagron	SyrSpend® SF pH4 neo	23J11-H01-00941	1
Fagron	SyrSpend® SF pH4 neo	24B28-H08-00941	1
Fagron	SyrSpend® SF Alka	2IL07-F05-381032	1
Fagron	SyrSpend® SF Alka	20B18F03369574	1
Fagron	SyrSpend® SF Alka	318828	1
Fagron	SyrSpend® SF Alka	379672	1
Fagron	SyrSpend® SF Alka	6369913	1
Fagron	SyrSpend® SF Alka	720026-0000	2
Fagron	SyrSpend® SF Alka	7-378133	1
Fagron	SyrSpend® SF Alka	802-3637809	1
Fagron	SyrSpend® SF Alka	B02-3637809	4
Fagron	SyrSpend® SF Alka	B04-3640507	1
Fagron	SyrSpend® SF Alka	B07-5261409	3
Fagron	SyrSpend® SF Alka	F01-3768209	2
Fagron	SyrSpend® SF Alka	F01-376829	2
Fagron	SyrSpend® SF pH4	F02-3723908	4
Fagron	SyrSpend® SF Alka	F02-3800301	1
Fagron	SyrSpend® SF pH4	F02-3834809	3
Fagron	SyrSpend® SF pH4	F03-3695400	1
Fagron	SyrSpend® SF Alka	F03-3695704	2
Fagron	SyrSpend® SF pH4	F03-3725107	1
Fagron	SyrSpend® SF Alka	F03-3788208	1
Fagron	SyrSpend® SF Alka	F0538103002	1
Fagron	SyrSpend® SF Alka	F06-3699103	3
Fagron	SyrSpend® SF Alka	F06-369913	1
Fagron	SyrSpend® SF Alka	F07-3699104	3
Fagron	SyrSpend® SF Alka	F07-3781303	1
Fagron	SyrSpend® SF Alka	F07-3788300	2
Fagron	SyrSpend® SF pH4	F08-3669902	1
Fagron	SyrSpend® SF pH4	F08-3669903	2
Fagron	SyrSpend® SF Alka	F08-3791401	2
Fagron	SyrSpend® SF pH4	F09-3670004	1
Fagron	SyrSpend® SF pH4	F10-3688704	2
Fagron	SyrSpend® SF Alka	F1137427009	3
Fagron	SyrSpend® SF Alka	F11-3742709	3
Fagron	SyrSpend® SF Alka	F12-3748002	1
Fagron	SyrSpend® SF pH4	FO3-3725107	1
Fagron	SyrSpend® SF Alka	FO4-3815505	1
Fagron	SyrSpend® SF Alka	FO6-3798904	1
Fargon / AHD	SyrSpend® SF Alka	20G03-F09-526400	1
Fargon/AHD	SyrSpend® SF Alka	18C13-B11	1
Fargon/Phönix	SyrSpend® SF Alka	20B25-F06-369913	2
Fargon	SyrSpend® SF Alka	19F12-B04-364057	1
Fargon	SyrSpend® SF Alka	21B26F07378133	1
Fiebig 16.01.13 ek: 4,18EUR	Amido de trigo	11350911	1
Fiebig	Amido de trigo	104A201028-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	SyrSpend® SF pH4	20F08-F03	1
Fiebig	Amido de milho	64A170123	1
Fischar/Gehe	SyrSpend® SF Alka	18L21-B11-359901	1
Fragon/ Noweda	SyrSpend® SF Alka	19F12-B04-364057	2
Fragron / Gehe	SyrSpend® SF Alka	20G03-F11-374279	1
Fresenius	Amido de trigo	13305103	1
Gehe	Amido de trigo	1028-01	1
Gehe	Amido de milho	16138505	1
Gehe	Amido de milho	17287302	1
Gehe	Amido de milho	17287305	1
Gehe	Amido de milho	18274802	2
Gehe	SyrSpend® SF Alka	18A26-B05-346410	1
Gehe	SyrSpend® SF Alka	18H01-B12-353473	1
Gehe	SyrSpend® SF pH4	18J16-B01-357703	3
Gehe	SyrSpend® SF Alka	18L21-B11	1
Gehe	Amido de milho	19187802	1
Gehe	SyrSpend® SF pH4	19A14-B07-362431	1
Gehe	Amido de milho	64A130304	1
Gutenberg-Apotheke	Amido de arroz	12360216	1
Kehr	Amido de trigo	104A160512	1
Kehr	SyrSpend® SF pH4	22L20-F03-384076	1
Kehr	SyrSpend® SF pH4	23E22-F01-384947	1
Klemk	Amido de trigo	104A160512	1
Klenk	Amido de trigo	101A201028-01	1
Klenk	Amido de trigo	1028-01	1
Klenk	Amido de trigo	104A101116	1
Klenk	Amido de arroz	104A120621	5
Klenk	Amido de arroz	104A130304	8
Klenk	Amido de trigo	104a141114	1
Klenk	Amido de arroz	104A141114	9
Klenk	Amido de trigo	104a160512	1
Klenk	Amido de trigo	104A160512	8
Klenk	Amido de trigo	104a171122	1
Klenk	Amido de trigo	104A171122	12
Klenk	Amido de trigo	104A19100101	1
Klenk	Amido de trigo	104A191001-01	3
Klenk	Amido de trigo	104A200107-01	2
Klenk	Amido de trigo	104A201028-01	4
Klenk	Amido de trigo	104A210720-01	1
Klenk	Amido de trigo	10720-01	1
Klenk	Amido de milho	10816-01	1
Klenk	Amido de trigo	10A160512	1
Klenk	Amido de trigo	10A201028-01	1
Klenk	Amido de trigo	191001-001	1
Klenk	Amido de milho	200427-001	2
Klenk	Amido de arroz	200921-002	1
Klenk	Amido de milho	220328A	1
Klenk	Amido de milho	4263535	1
Klenk	Amido de milho	427-01	1
Klenk	Amido de arroz	64A080218	5
Klenk	Amido de arroz	64a130304	1
Klenk	Amido de arroz	64A130304	18
Klenk	Amido de milho	64A170123	31
Klenk	Amido de milho	64A181203	15
Klenk	Amido de milho	64A20042701	2
Klenk	Amido de milho	64A200427-01	17
Klenk	Amido de milho	64-A-200427-01	1
Klenk	Amido de milho	64A21081601	1
Klenk	Amido de milho	64A210816-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Amido de milho	6A181203	1
Klenk	Fécula de batata	80919-01	1
Klenk	Amido de arroz	84A130304	1
Klenk	Amido de arroz	84A141114	4
Klenk	Amido de arroz	84A180522	2
Klenk	Amido de trigo	91001-01	1
Klenk	Amido de arroz	94A100122	1
Klenk	Fécula de batata	94A110512	1
Klenk	Amido de arroz	94A130304	5
Klenk	Fécula de batata	94a170123	1
Klenk	Fécula de batata	94A170123	4
Klenk	Fécula de batata	94A180919	1
Klenk	Fécula de batata	94A180919-01	3
Klosterring	Amido de trigo	15421507	1
Koisser	Amido de arroz	WE07032013	1
Krieger	SyrSpend® SF Alka	22B04-F06-381564	1
Nachprüfung	Amido de trigo	3082019-1	1
Nachprüfung	Amido de arroz	3709E01116	1
Nachprüfung	Amido de milho	AP200525-12	1
Noweda/Hedinger	SyrSpend® SF pH4	18J16-B01-357703	1
Noweda	Amido de trigo	104A221027-01	1
Noweda	Amido de arroz	14011621	1
Noweda	Amido de arroz	14023203	1
noweda	SyrSpend® SF pH4	15I22-B02-52176	1
Noweda	SyrSpend® SF Alka	18L21-B11-359901	1
Noweda	Amido de milho	20004426006	1
Noweda	Amido de milho	20004426018	1
Noweda	Amido de arroz	20004428009	1
Noweda	SyrSpend® SF Alka	20B25-F07	1
Noweda	SyrSpend® SF pH4	2209-F03-383490	1
Noweda	SyrSpend® SF Alka	22A12-F22-382195	1
Noweda	SyrSpend® SF pH4	22I09-F02-383489	1
Noweda	SyrSpend® SF pH4	22I09-F03-383490	1
Noweda	SyrSpend® SF Alka	22J04-F02-383639	1
Noweda	SyrSpend® SF Alka	22J31-F01-526993	1
Noweda	SyrSpend® SF Alka	22JO4-FO6-383652	1
Phoenix	SyrSpend® SF pH4	16J10-B03-330757	3
Phoenix	SyrSpend® SF pH4	18H30-B02-355226	1
Phoenix	SyrSpend® SF pH4	18J25-B15-357803	1
Phoenix	SyrSpend® SF Alka	18L21-B11-359901	6
Phoenix	SyrSpend® SF Alka	19D29-B07-362182	4
Phoenix	SyrSpend® SF Alka	19D29-B11-363786	3
Phoenix	SyrSpend® SF Alka	FO3-3788208	1
Phönix/Fagon	SyrSpend® SF Alka	17D11-B04-332593	1
Phönix	Amido de trigo	104A191001-01	1
PHönix	Amido de trigo	104A210720-01	1
PHÖNIX	Amido de trigo	16162905	1
Phönix	SyrSpend® SF Alka	18B13-B11-350851	1
Phönix	SyrSpend® SF Alka	18H01-B12-353473	9
Phönix	SyrSpend® SF pH4	18H30-B02-355226	8
Phönix	SyrSpend® SF Alka	19F12-B04-364057	1
Phönix	SyrSpend® SF Alka	21F08-F03378828	1
Phönix	SyrSpend® SF Alka	21L07-F05	3
Phönix	SyrSpend® SF Alka	22B04-F04-381555	8
phönix	Amido de arroz	84a141114	1
Phönix	Amido de arroz	84A141114	2
Sanacorp	Amido de milho	18274808	1
Sanacorp	SyrSpend® SF Alka	21F08-F03-378828	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	SyrSpend® SF Alka	21F08-F03-378828210166	1
Sanacorp	SyrSpend® SF Alka	22804-F07	1
Sanacorp	SyrSpend® SF Alka	22J04-F11-383746	2
Sanacorp	SyrSpend® SF Alka	23A18-F07-384725	2
Sanacorp	SyrSpend® SF pH4	23E22-F02-384949	1
Sanacorp	SyrSpend® SF pH4 neo	24H06-H07-00941	1
Sanacorp	Amido de milho	64A181203	1
Sanacorp	Amido de arroz	84A141114	1
sanacorp	Amido de arroz	94A130304	1
Spinnrad GmbH	Amido de milho	519408192	1
VDL;03.03.15;3,04EUR	Amido de arroz	14011627	1
VDL;3,03EUR;11.06.15	Amido de arroz	14011630	1

- 234 230 spectra from 1515 *Apo-Ident* customers from a total of 48 721 batches from a further 715 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Amido* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Amido* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1860	0	151 102
Type B	0	1550	0	200 520
Type C	0	1836	1	234 200

The substance/substance group *Amido* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.6774 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6129 %)
Type C	100.0000 % (> 99.9005 %)	99.9456 % (> 99.7823 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20790	22450	8,42	55,22
20996	20996	0,00	69,99
21447	21447	0,00	52,38
21827	22450	5,88	58,62
21965	22449	6,69	73,62
21973	22450	7,82	58,65
22246	22450	11,25	56,17
22449	22449	0,00	69,11
22450	22450	0,00	60,73
22496	22496	0,00	40,22
22497	22496	2,10	40,49
22585	25767	8,40	52,41
22719	22719	0,00	32,16
23219	23220	7,25	38,42
23220	23220	0,00	45,49
23448	24112	16,67	52,30
23449	24112	16,23	51,72
23510	21447	12,60	59,20
23750	23750	0,00	54,00
23923	22449	7,15	71,27
24112	24112	0,00	61,76
24290	24112	7,29	60,22
24361	24361	0,00	59,51
25080	25080	0,00	29,89
25363	24112	17,20	48,27
25369	22496	9,96	38,61
25382	22449	9,77	68,40
25383	22450	9,33	48,80
25534	25534	0,00	34,02
25755	25755	0,00	41,97
25767	25767	0,00	50,42
26568	22496	15,58	35,86
26613	22496	5,72	39,73
26677	22496	9,73	37,72
27029	24112	24,85	46,06
27030	22496	18,08	38,51
27056	22496	14,41	44,79
27107	27107	0,00	54,88
27180	22496	11,68	38,34
27192	22496	14,61	43,53
27321	27321	0,00	71,57
27324	27324	0,00	55,98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amifampridina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20317-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amifampridina; Amifampridinum

Special notes

When selecting the *Amifampridina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Amifampridina	6	7	45

Second-stage model

For differentiation of the substance/substance group *Amifampridina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Amifampridina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	123,57	–
⋮	⋮	⋮
Citrato de sódio	>50	178,69
Heparina sódica	>50	191,30
Capsaicina	>50	241,34
Sacarose	>50	488,81
Levocarnitina	>50	562,85
Cloridrato de oxibutinina	>50	583,57
Alfaestradiol	>50	594,71
Prednicarbato	>50	629,63
Cloridrato de quinina di-hidratado	>50	656,43
Piridoxal-5-fosfato	>50	692,14
Tetracaína	>50	802,23
Metoxisaleno	>50	927,92
Triclosan	>50	952,34
Cloridrato de ciprofloxacina	>50	1138,74
Acetato de ciproterona	>50	1322,58
Acetato de noretisterona	>50	1461,75
Cloridrato de amitriptilina	>50	2526,08
Valina	>50	3980,96

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Amifampridina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Amifampridina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Amifampridina	17251208	24177	40	20171117
Caelo	Amifampridina	19180701	25392	40	2104347

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amifampridina	13F05-N01	20901	41	20130606
Fagron	Amifampridina	16A22-B04-317264	22321	60	20160204
Fagron	Amifampridina	19K01-F01-366966	25175	40	20191219
Inresa	Amifampridina	33-15-IV-56P2749B	22848	40	20160822

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 261 spectra of 6 reference samples from the substance/substance group *Amifampridina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 701 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 350 spectra of 11 reference samples from the substance/substance group *Amifampridina*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Amifampridina	22000776004	26308	40
Euro OTC	Amifampridina	2108004	25818	50
Euro OTC	Amifampridina	2201034	25951	40
Fagron	Amifampridina	17J11-B01-340962	23766	40
Fagron	Amifampridina	22A22-B04-219578	26136	40
Fagron	Amifampridina	24G03-B01-001048	27378	40
Inresa	Amifampridina	33-16-I-77P3018	23723	40
Caelo	Amifampridina	22000776004	26308SI	20
Euro OTC	Amifampridina	2108004	25818SI	10
Euro OTC	Amifampridina	2201034	25951SI	10
Fagron	Amifampridina	22A22-B04-219578	26136SI	20

- 201 734 spectra from a total of 4038 batches from further 842 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 98 spectra from 22 *Apo-Ident* customers from 47 batches from the substance/substance group *Amifampridina*.
- Among them are spectra of independent samples from 45 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amifampridina	B02-2237706	1
Caelo	Amifampridina	13f05-n01	1
Caelo	Amifampridina	17251206	6
Caelo	Amifampridina	17251207	1
Caelo	Amifampridina	17251209	1
Caelo	Amifampridina	17251210	4
Caelo	Amifampridina	19180702	3
Caelo	Amifampridina	19180703	1
Caelo	Amifampridina	193070001	2
Caelo	Amifampridina	193070002	2
Caelo	Amifampridina	19307001	1
Caelo	Amifampridina	21003139002	2
Caelo	Amifampridina	22000776002	1
Caelo	Amifampridina	22000776003	2
Caelo	Amifampridina	33-15-IV-56P2749	1
Caelo	Amifampridina	33-15IV-56P2749B	1
Caesar & Loretz GmbH...	Amifampridina	21003139002	1
Caesar & Loretz GmbH/Gehe	Amifampridina	22000776002	1
Caesar & Loretz GmbH	Amifampridina	19180702	1
Fagron	Amifampridina	11/14-N03	1
Fagron	Amifampridina	11K07-N02	1
Fagron	Amifampridina	13F07-NU7	1
Fagron	Amifampridina	13K14-M01	1
Fagron	Amifampridina	13L12-M03	1
Fagron	Amifampridina	13L12-M06	2
Fagron	Amifampridina	14H11-B06	3
Fagron	Amifampridina	14H11-B06-298447	2
Fagron	Amifampridina	15B20-B02	2
Fagron	Amifampridina	16D05-B01	1
Fagron	Amifampridina	16D05-B01-318216	1
Fagron	Amifampridina	16K15-B03-330546	1
Fagron	Amifampridina	17J11-B01-343013	1
Fagron	Amifampridina	17L19-B02-352347	1
Fagron	Amifampridina	18G04-B14-353053	3
Fagron	Amifampridina	20J13-F01	1
Fagron	Amifampridina	21C17-F01-377439	1
Gehe	Amifampridina	13F07-N07	1
Inresa Arzneimittel GmbH	Amifampridina	33-16-I-77P3018/1307	1
Inresa	Amifampridina	33-15-IV-56P2749	2
Inresa	Amifampridina	33-15-IV-56P2749B	3
Inresa	Amifampridina	33-15-IV-56P2749B/22	3
Inresa	Amifampridina	33-16-I-77P3018	3
Inresa	Amifampridina	33-16-I-77P3018/1307	2
Inresa	Amifampridina	3316I77P301816022018	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Inresa	Amifampridina	508670001	1
inresa	Amifampridina	58010001	1
inresa	Amifampridina	580710001	2
Inresa	Amifampridina	580710001	9
inresa	Amifampridina	58710001	2
inresa	Amifampridina	631350001	1
Inresa	Amifampridina	631350001	3
Inresa	Amifampridina	63150001	1
Phönix	Amifampridina	22000776003	1
Phönix	Amifampridina	23000580001	1
Sanacorp	Amifampridina	17251209	2
Sanacorp	Amifampridina	20L14-F03-376279	1

- 235 969 spectra from 1515 *Apo-Ident* customers from a total of 49 212 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Amifampridina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Amifampridina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	261	0	152 701
Type B	0	350	0	201 734
Type C	0	98	0	235 969

The substance/substance group *Amifampridina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7011 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.8776 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20901	25392	9,56	316,39
22321	25392	9,12	316,81
22848	25392	12,28	315,05
24177	25392	6,47	318,61
25175	25392	6,45	317,91
25392	25392	0,00	320,92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amoxicilina tri-hidratada**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006096-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amoxicilina tri-hidratada; Amoxicillinum trihydricum

Special notes

When selecting the *Amoxicilina tri-hidratada* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Amoxicilina tri-hidratada	5	2	2

Second-stage model

For differentiation of the substance/substance group *Amoxicilina tri-hidratada* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Amoxicilina tri-hidratada* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	63,40	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Amoxicilina tri-hidratada* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Amoxicilina tri-hidratada*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Amoxicilina tri-hidratada	2301017	26570	40	20230223*
Euro OTC	Amoxicilina tri-hidratada	2301052	26571	40	20230228*
Euro OTC	Amoxicilina tri-hidratada	2305004	26764	40	20230703*
Euro OTC	Amoxicilina tri-hidratada	2306006	26765	40	20230712*
Fagron	Amoxicilina tri-hidratada	23F29-F01-384940	27023	40	20230703

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Amoxicilina tri-hidratada*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 5 reference samples from the substance/substance group *Amoxicilina tri-hidratada*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Amoxicilina tri-hidratada	2304002	26662	40
Gatt-Koller	Amoxicilina tri-hidratada	23J00336	26624	40
Euro OTC	Amoxicilina tri-hidratada	2301017	26570SI†	20
Euro OTC	Amoxicilina tri-hidratada	2301052	26571SI†	20
Gatt-Koller	Amoxicilina tri-hidratada	23J00336	26624SI	20

- 201 944 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Amoxicilina tri-hidratada*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amoxicilina tri-hidratada	221213182	2
	Amoxicilina tri-hidratada	2305004-01	2

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Amoxicilina tri-hidratada* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Amoxicilina tri-hidratada* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	136	4	201 944
Type C	0	4	0	236 063

The substance/substance group *Amoxicilina tri-hidratada* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	97.1429 % (> 95.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26570	26570	0,00	135,45
26571	26571	0,00	134,35
26764	26764	0,00	134,51
26765	26765	0,00	134,23
27023	26570	12,18	134,95

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Anfotericina B**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20933-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Anfotericina B; Amphotericinum B

Special notes

When selecting the *Anfotericina B* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Anfotericina B	6	9	8

Second-stage model

For differentiation of the substance/substance group *Anfotericina B* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Anfotericina B* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	43,48	18,52
Bacitracina	76,60	16,74
⋮	⋮	⋮
Nistatina	>50	20,95
Cianocobalamina	>50	26,46
Sulfato de colistina	>50	26,65
Riboflavina	>50	47,83
Pantotenato de cálcio	>50	59,20
Estradiol hemi-hidratado	>50	62,76
Levedura de selênio	>50	63,29
Vitamina E acetato pó 50%	>50	65,58
Triancinolona	>50	72,82
Glicerofosfato de cálcio	>50	78,15
Metilcobalamina	>50	79,92
Estriol	>50	80,79
Gelatina, branca	>50	83,75
Bromidrato de hioscina	>50	128,71
Carmelose sódica	>50	129,08
SyrSpend® SF Alka	>50	142,16
Tosilcloramida sódica	>50	146,43
SyrSpend® SF pH4 neo	>50	149,63
Amido de arroz	>50	186,60
Ácido oxálico	>50	240,01
Amido de milho	>50	244,43
SyrSpend® SF pH4	>50	298,91
Goma arábica, dispersão seca	>50	343,80
Amido de trigo	>50	363,92
Maltodextrina	>50	365,91
Fécula de batata	>50	382,10
Frutose	>50	479,71

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Anfotericina B* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Anfotericina B*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Anfotericina B	1305033-02	20933	40	1403224
Euro OTC	Anfotericina B	1512026-01	22813	40	20160121
Euro OTC	Anfotericina B	2008028	25397	40	20200930*
Euro OTC	Anfotericina B	2105013	25761	50	20210826*
Fagron	Anfotericina B	13I16-N02	21338	40	1508271
Fagron	Anfotericina B	13I16-N02	21951	60	20130911
Fagron	Anfotericina B	16L06-B04-333234	23530	40	20170103

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 310 spectra of 7 reference samples from the substance/substance group *Anfotericina B*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 652 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 420 spectra of 12 reference samples from the substance/substance group *Anfotericina B*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Anfotericina B	1803036	24065	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Anfotericina B	1903002	24614	40
Euro OTC	Anfotericina B	2202018	26031	40
Euro OTC	Anfotericina B	2203033	26089	40
Euro OTC	Anfotericina B	2209011	26433	40
Euro OTC	Anfotericina B	2301050	26939	40
Euro OTC	Anfotericina B	2401018	27157	40
Fagron	Anfotericina B	20G16-F06-373576	25715	50
Fagron	Anfotericina B	22C16-B01-227326	26538	40
Euro OTC	Anfotericina B	2202018	26031SI	10
Euro OTC	Anfotericina B	2203033	26089SI	20
Fagron	Anfotericina B	22C16-B01-227326	26538SI	20

- 201 664 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 21 spectra from 12 *Apo-Ident* customers from 9 batches from the substance/substance group *Anfotericina B*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Anfotericina B	1305033-03	12
Euro OTC	Anfotericina B	1803036-01	1
Euro OTC	Anfotericina B	1903002-01	2
Fagron	Anfotericina B	16D05-B04	1
Fagron	Anfotericina B	16106-b04-333234	1
Fagron	Anfotericina B	18Job-B02-358370	1
Fagron	Anfotericina B	20C03-F01-371264	1
Fagron	Anfotericina B	20F10-F03-372701	1
Fagron	Anfotericina B	5173	1

- 236 046 spectra from 1515 *Apo-Ident* customers from a total of 49 249 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Anfotericina B* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Anfotericina B* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	420	0	201 664
Type C	0	21	0	236 046

The substance/substance group *Anfotericina B* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5714 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 71.4286 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20933	20933	0,00	77,64
21338	21338	0,00	80,77
21951	21338	10,59	82,08
22813	20933	9,11	76,60
23530	20933	13,12	77,26
25397	25397	0,00	78,29
25761	25761	0,00	78,46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Arginina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20391-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Arginina; Argininum

Special notes

When selecting the *Arginina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Arginina	8	10	61

Second-stage model

For differentiation of the substance/substance group *Arginina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Arginina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Trometamol	79,41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Arginina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Arginina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Arginina	1604003	22514	40	20160425*
Euro OTC	Arginina	1608031	22801	40	20160916*
Euro OTC	Arginina	1702014	23154	40	20170316*
Euro OTC	Arginina	2001001	25092	40	20200122*
Euro OTC	Arginina	2208024	26533	40	20230119*
Euro OTC	Arginina	2208024	26533SI	20	20230119*
Fagron	Arginina	13J28-B02	21226	40	AR-15-FG-008045-01
Fagron	Arginina	16H24-B04-335673	23748	40	20161010
Fagron	Arginina	21L16-B02-220332	26132	40	20220401
Fagron	Arginina	21L16-B02-220332	26132SI	20	20220401

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 10 reference samples from the substance/substance group *Arginina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 420 spectra of 11 reference samples from the substance/substance group *Arginina*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Arginina	1710010	23774	40
Euro OTC	Arginina	1806010	24154	40
Euro OTC	Arginina	1902024	24478	40
Euro OTC	Arginina	1909005	24856	40
Euro OTC	Arginina	2008003	25477	40
Euro OTC	Arginina	2107003	25774	50
Euro OTC	Arginina	2203019	26030	40
Euro OTC	Arginina	2307009	26867	40
Euro OTC	Arginina	2402021	27141	40
Fagron	Arginina	24A10-B07-235268	27170	40
Euro OTC	Arginina	2203019	26030SI	10

- 201 664 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 119 spectra from 29 *Apo-Ident* customers from 63 batches from the substance/substance group *Arginina*.

- Among them are spectra of independent samples from 61 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Arginina	21L-16-B02-220332	4
	Arginina	22G19-B03-221821	2
Caelo	Arginina	13J28-B02-290463	1
Caelo	Arginina	14124-B08-303720	1
Caelo	Arginina	15C10-B03-314547	1
Caelo	Arginina	15C10-B03-318785	1
Caelo	Arginina	17G10-B07-347888	1
Euro OTC	Arginina	1105040-01	1
Euro OTC	Arginina	1604003-01	1
Euro OTC	Arginina	1710010-01	2
Euro OTC	Arginina	17122746	1
Euro OTC	Arginina	1902024-01	6
Euro OTC	Arginina	1909005-01	5
Euro OTC	Arginina	2001001-01	3
Euro OTC	Arginina	2001001-1	1
Euro OTC	Arginina	2008003-01	2
Euro OTC	Arginina	2009040-01	3
Euro OTC	Arginina	20113317	1
Euro OTC	Arginina	L1206006-01	1
Fagron	Arginina	12C21-N04	1
Fagron	Arginina	13031801	1
Fagron	Arginina	13F14-N02	2
Fagron	Arginina	13J28-B02-290463	6
Fagron	Arginina	14/24-B08-303720	4
Fagron	Arginina	14/24-B08-303721	2
Fagron	Arginina	14/24-B08-303901	1
Fagron	Arginina	14062019	1
Fagron	Arginina	14092035	2
Fagron	Arginina	1424-B08-303720	1
Fagron	Arginina	14B25-B04	2
Fagron	Arginina	14B25-B04-295749	1
Fagron	Arginina	14I24-B08-303901	1
Fagron	Arginina	14I24-B-303720	1
Fagron	Arginina	15102258	1
Fagron	Arginina	15C10-B03-318784	1
Fagron	Arginina	16032361	1
Fagron	Arginina	16D11-B01-322156	1
Fagron	Arginina	16D11-B01-323566	2
Fagron	Arginina	16H24-B04-328914	1
Fagron	Arginina	16H24-B04-331399	1
Fagron	Arginina	16H24-B04-334063	2
Fagron	Arginina	16H24-B04-335673	3
Fagron	Arginina	16H24-B04-335674	8
Fagron	Arginina	16H24-B04-341855	1
Fagron	Arginina	17022585	1
Fagron	Arginina	17G10-B07	1
Fagron	Arginina	17G10-B07-345399	2
Fagron	Arginina	17G10-B07-347888	1
Fagron	Arginina	17G10-B07-349772	3
Fagron	Arginina	17G10-B07-352495	1
Fagron	Arginina	17G10-B07-354908	1
Fagron	Arginina	18072859	1
Fagron	Arginina	18J04-B03-357823	5
Fagron	Arginina	18J04-B03-357824	2
Fagron	Arginina	19G04-B05-363253	1
Fagron	Arginina	19g04-b05-364722	1
Fagron	Arginina	19G04-B05-364722	1
Fagron	Arginina	20A16-F07-368384	2
Fagron	Arginina	20E08-F09-370773	1
Fagron	Arginina	21F14-B11-213620	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Arginina	701743-0006	1
Fagron	Arginina	B05-3647202	1
Fargon	Arginina	121429	1
GEHE	Arginina	17G10-B07-341856	2
Phönix	Arginina	L1302006-01	1

- 235 948 spectra from 1515 *Apo-Ident* customers from a total of 49 196 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Arginina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Arginina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	420	0	201 664
Type C	0	119	0	235 948

The substance/substance group *Arginina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5714 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 94.9580 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21226	21226	0,00	168,30
22514	22514	0,00	155,77
22801	22801	0,00	143,97
23154	23154	0,00	149,80
23748	25092	5,99	165,86
25092	25092	0,00	170,16
26132	25092	5,84	169,27
26533	26533	0,00	165,17

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ascorbato de cálcio di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20393-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ascorbato de cálcio di-hidratado; Calcii ascorbas dihydricum

Special notes

When selecting the *Ascorbato de cálcio di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ascorbato de cálcio di-hidratado	9	14	18

Second-stage model

For differentiation of the substance/substance group *Ascorbato de cálcio di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ascorbato de cálcio di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	84,23	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ascorbato de cálcio di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ascorbato de cálcio di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ascorbato de cálcio di-hi…	13105624	21313	40	20130620
Caelo	Ascorbato de cálcio di-hi…	163111	23060	40	20161207*
Caelo	Ascorbato de cálcio di-hi…	16311101	23518	40	20161207
Caelo	Ascorbato de cálcio di-hi…	20003812	25625	40	20201211*
Euro OTC	Ascorbato de cálcio di-hi…	1612003	22916	40	20170110*
Euro OTC	Ascorbato de cálcio di-hi…	1709005	23609	40	20170914*
Euro OTC	Ascorbato de cálcio di-hi…	1709004	23611	40	20170914*
Euro OTC	Ascorbato de cálcio di-hi…	1801010	23884	40	20180115*
Euro OTC	Ascorbato de cálcio di-hi…	2201040	26093	40	20220211*
Euro OTC	Ascorbato de cálcio di-hi…	2201040	26093SI	20	20220211*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Ascorbato de cálcio di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 582 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 590 spectra of 16 reference samples from the substance/substance group *Ascorbato de cálcio di-hidratado*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ascorbato de cálcio di-hi…	183226	24373	40
Caelo	Ascorbato de cálcio di-hi…	19000538	25223	40
Caelo	Ascorbato de cálcio di-hi…	22000185	26014	30
Euro OTC	Ascorbato de cálcio di-hi…	1607033-01	22812	40
Euro OTC	Ascorbato de cálcio di-hi…	1807032	24194	40
Euro OTC	Ascorbato de cálcio di-hi…	1901003	24470	40
Euro OTC	Ascorbato de cálcio di-hi…	1904010	24626	40
Euro OTC	Ascorbato de cálcio di-hi…	1910003	24979	40
Euro OTC	Ascorbato de cálcio di-hi…	2003025	25149	40
Euro OTC	Ascorbato de cálcio di-hi…	2007012	25336	40
Euro OTC	Ascorbato de cálcio di-hi…	2101005	25538	40
Euro OTC	Ascorbato de cálcio di-hi…	2105006	25768	50
Euro OTC	Ascorbato de cálcio di-hi…	2305017	26881	40
Euro OTC	Ascorbato de cálcio di-hi…	2403007	27345	40
Caelo	Ascorbato de cálcio di-hi…	22000185	26014SI	10
Euro OTC	Ascorbato de cálcio di-hi…	2305017	26881SI	20

- 201 494 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 28 spectra from 12 *Apo-Ident* customers from 21 batches from the substance/substance group *Ascorbato de cálcio di-hidratado*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ascorbato de cálcio di-hi…	2305017-01	2
Arktis	Ascorbato de cálcio di-hi…	7339/4617	1
Arktis	Ascorbato de cálcio di-hi…	733P/1518	1
Burton Feingold	Ascorbato de cálcio di-hi…	L008415	1
Caelo	Ascorbato de cálcio di-hi…	13105608	1
Caelo	Ascorbato de cálcio di-hi…	14340907	1
Caelo	Ascorbato de cálcio di-hi…	15324702	1
Caelo	Ascorbato de cálcio di-hi…	15324708	2
Caelo	Ascorbato de cálcio di-hi…	16311101	1
Caelo	Ascorbato de cálcio di-hi…	16311105	1
Euro OTC	Ascorbato de cálcio di-hi…	1709004-01	1
Euro OTC	Ascorbato de cálcio di-hi…	1709005	1
Euro OTC	Ascorbato de cálcio di-hi…	1801010	1
Euro OTC	Ascorbato de cálcio di-hi…	1901003-01	1
Euro OTC	Ascorbato de cálcio di-hi…	1904010-01	3
Euro OTC	Ascorbato de cálcio di-hi…	1910003-01	3
Euro OTC	Ascorbato de cálcio di-hi…	2007012-01	2
Euro OTC	Ascorbato de cálcio di-hi…	2105006-01	1
Euro OTC	Ascorbato de cálcio di-hi…	220104001	1
Farmalabor / Farmalabor	Ascorbato de cálcio di-hi…	P1104931-000A	1
Gatt-Koller	Ascorbato de cálcio di-hi…	1900123	1

- 236 039 spectra from 1515 *Apo-Ident* customers from a total of 49 237 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ascorbato de cálcio di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ascorbato de cálcio di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	590	0	201 494
Type C	0	28	0	236 039

The substance/substance group *Ascorbato de cálcio di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9831 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 78.5714 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21313	23060	9,77	202,22
22916	22916	0,00	200,63
23060	23060	0,00	199,49
23518	25625	4,00	198,10
23609	23609	0,00	199,49
23611	23611	0,00	198,66
23884	23884	0,00	198,08
25625	25625	0,00	200,46
26093	26093	0,00	202,84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ascorbato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20520-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ascorbato de sódio; Natrii ascorbas

Special notes

When selecting the *Ascorbato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ascorbato de sódio	8	53	34

Second-stage model

For differentiation of the substance/substance group *Ascorbato de sódio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ascorbato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloreto de alumínio hexa-hidratado	88,66	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ascorbato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ascorbato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ascorbato de sódio	15429905	22899	40	20160118
Caelo	Ascorbato de sódio	182620	24386	40	20181112*
Caelo	Ascorbato de sódio	20001049	25554	40	20200731*
Euro OTC	Ascorbato de sódio	1406018-01	21583	60	1411165
Euro OTC	Ascorbato de sódio	1406018-01	21789	60	20140724
Euro OTC	Ascorbato de sódio	1507030	21853	60	20150811*
Euro OTC	Ascorbato de sódio	1506018	21865	60	20150706*
Euro OTC	Ascorbato de sódio	1510017	21946	60	20151102*
Euro OTC	Ascorbato de sódio	1601007	22304	60	20160120*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 9 reference samples from the substance/substance group *Ascorbato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 482 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2419 spectra of 63 reference samples from the substance/substance group *Ascorbato de sódio*.

- Among them are spectra of independent samples from 53 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ascorbato de sódio	162857	22761	40
Caelo	Ascorbato de sódio	172235	23809	40
Caelo	Ascorbato de sódio	180326	24029	40
Caelo	Ascorbato de sódio	191393	24751	40
Caelo	Ascorbato de sódio	192304	24896	40
Caelo	Ascorbato de sódio	22002242	26365	30
Caelo	Ascorbato de sódio	23002840	27103	40
Caelo	Ascorbato de sódio	24000403	27245	40
Caelo	Ascorbato de sódio	24002134	27448	40
Euro OTC	Ascorbato de sódio	1604001	22524	40
Euro OTC	Ascorbato de sódio	1607044	22690	40
Euro OTC	Ascorbato de sódio	1611015	22864	40
Euro OTC	Ascorbato de sódio	1701054	23134	40
Euro OTC	Ascorbato de sódio	1703012	23152	40
Euro OTC	Ascorbato de sódio	1705013	23430	40
Euro OTC	Ascorbato de sódio	1705014	23432	40
Euro OTC	Ascorbato de sódio	1803005	24069	40
Euro OTC	Ascorbato de sódio	1807043	24149	40
Euro OTC	Ascorbato de sódio	1811002	24337	40
Euro OTC	Ascorbato de sódio	1902021	24460	40
Euro OTC	Ascorbato de sódio	1906005	24786	40
Euro OTC	Ascorbato de sódio	1906004	24807	40
Euro OTC	Ascorbato de sódio	1908026	24930	40
Euro OTC	Ascorbato de sódio	2003024	25164	40
Euro OTC	Ascorbato de sódio	2007008	25320	40
Euro OTC	Ascorbato de sódio	2007009	25321	40
Euro OTC	Ascorbato de sódio	2007010	25322	40
Euro OTC	Ascorbato de sódio	2007011	25340	40
Euro OTC	Ascorbato de sódio	2104010	25670	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ascorbato de sódio	2105016	25710	50
Euro OTC	Ascorbato de sódio	2201001	25963	40
Euro OTC	Ascorbato de sódio	2201002	25965	40
Euro OTC	Ascorbato de sódio	2205026	26187	40
Euro OTC	Ascorbato de sódio	2205025	26193	40
Euro OTC	Ascorbato de sódio	2208013	26274	40
Euro OTC	Ascorbato de sódio	2208014	26278	39
Euro OTC	Ascorbato de sódio	2211010	26420	40
Euro OTC	Ascorbato de sódio	2211011	26441	40
Euro OTC	Ascorbato de sódio	2308007	26933	40
Euro OTC	Ascorbato de sódio	2308009	26935	40
Euro OTC	Ascorbato de sódio	2308008	26936	40
Euro OTC	Ascorbato de sódio	2402016	27197	40
Euro OTC	Ascorbato de sódio	2402011	27199	40
Euro OTC	Ascorbato de sódio	2402014	27201	40
Euro OTC	Ascorbato de sódio	2402015	27202	40
Euro OTC	Ascorbato de sódio	2402001	27270	40
Euro OTC	Ascorbato de sódio	2402002	27271	40
Euro OTC	Ascorbato de sódio	2402003	27272	40
Euro OTC	Ascorbato de sódio	2402010	27273	40
Euro OTC	Ascorbato de sódio	2402005	27356	40
Euro OTC	Ascorbato de sódio	2402004	27357	40
Euro OTC	Ascorbato de sódio	2402006	27358	40
Euro OTC	Ascorbato de sódio	2402007	27359	40
Caelo	Ascorbato de sódio	22002242	26365SI	20
Euro OTC	Ascorbato de sódio	1906004	24935	40
Euro OTC	Ascorbato de sódio	1902021	24943	40
Euro OTC	Ascorbato de sódio	1906005	24976	40
Euro OTC	Ascorbato de sódio	2201001	25963SI	40
Euro OTC	Ascorbato de sódio	2201002	25965SI	40
Euro OTC	Ascorbato de sódio	2205026	26187SI	20
Euro OTC	Ascorbato de sódio	2205025	26193SI	20
Euro OTC	Ascorbato de sódio	2208013	26274SI	20
Euro OTC	Ascorbato de sódio	2208014	26278SI	20

- 199 665 spectra from a total of 3992 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 43 spectra from 16 *Apo-Ident* customers from 34 batches from the substance/substance group *Ascorbato de sódio*.
- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Ascorbato de sódio	14079404	1
Caelo	Ascorbato de sódio	15180505	1
Caelo	Ascorbato de sódio	15429917	1
Caelo	Ascorbato de sódio	1604001-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ascorbato de sódio	1628505	1
Caelo	Ascorbato de sódio	16285710	1
Caelo	Ascorbato de sódio	17223504	1
Caelo	Ascorbato de sódio	17356201	1
Caelo	Ascorbato de sódio	27091302	1
Caesar & Loretz GmbH/gehe	Ascorbato de sódio	19139304	1
Caesar & Loretz GmbH	Ascorbato de sódio	18262001	1
Caesar & Loretz GmbH	Ascorbato de sódio	18262009	1
Caesar & Loretz GmbH	Ascorbato de sódio	21001574004	2
Caesar & Loretz GmbH	Ascorbato de sódio	21003620003	1
Euro OTC	Ascorbato de sódio	11081401	1
Euro OTC	Ascorbato de sódio	11121301	1
Euro OTC	Ascorbato de sódio	12061407	1
Euro OTC	Ascorbato de sódio	1210026-01	1
Euro OTC	Ascorbato de sódio	13031402	1
Euro OTC	Ascorbato de sódio	13051406	1
Euro OTC	Ascorbato de sódio	16091301	1
Euro OTC	Ascorbato de sódio	170105401	1
Euro OTC	Ascorbato de sódio	1703012-01	1
Euro OTC	Ascorbato de sódio	200708-01	1
Euro OTC	Ascorbato de sódio	20091303	1
Euro OTC	Ascorbato de sódio	2208013-01	2
Euro OTC	Ascorbato de sódio	28081304	1
Euro OTC	Ascorbato de sódio	4021401	1
Euro OTC	Ascorbato de sódio	7011405	1
Euro OTC	Ascorbato de sódio	L1308005-01	1
Fagron	Ascorbato de sódio	12L27-N03	1
Fagron	Ascorbato de sódio	13C15-N01	1
Gatt-Koller	Ascorbato de sódio	1802317	3
Pharma Greven	Ascorbato de sódio	HPN1904025	6

- 236 024 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ascorbato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ascorbato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	2419	0	199 665
Type C	0	43	0	236 024

The substance/substance group *Ascorbato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.7520 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.0465 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21583	21583	0,00	158,39
21789	21865	4,16	181,17
21853	21853	0,00	175,26
21865	21865	0,00	177,93
21946	21946	0,00	171,91
22304	22304	0,00	185,95
22899	22304	4,37	187,01
24386	24386	0,00	185,12
25554	25554	0,00	186,34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Aspartato de ornitina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20842-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Aspartato de ornitina; Ornithini aspartas; Ornitina aspartato

Special notes

When selecting the *Aspartato de ornitina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Aspartato de ornitina	9	4	0

Second-stage model

For differentiation of the substance/substance group *Aspartato de ornitina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Aspartato de ornitina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	80,14	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Aspartato de ornitina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Aspartato de ornitina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Aspartato de ornitina	1312030-01	21710	60	1506280
Euro OTC	Aspartato de ornitina	1611018	22924	40	20161213*
Euro OTC	Aspartato de ornitina	1611018-01	23198	40	20161213
Euro OTC	Aspartato de ornitina	2301047	26592	40	20230307*
Euro OTC	Aspartato de ornitina	2307023	26877	40	20230804*
Euro OTC	Aspartato de ornitina	2404004	27404	40	20241104*
Fagron	Aspartato de ornitina	14A20-B07-296093	21694	45	1506279
Fagron	Aspartato de ornitina	14I24-B04-307758	22599	40	20141110
Fagron	Aspartato de ornitina	14I24-B04-307758	22600	40	20141110
Fagron	Aspartato de ornitina	17I21-B05-342561	23864	40	1804455

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 425 spectra of 10 reference samples from the substance/substance group *Aspartato de ornitina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 537 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Aspartato de ornitina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Aspartato de ornitina	1711015	23899	40
Euro OTC	Aspartato de ornitina	1805026	24125	40
Euro OTC	Aspartato de ornitina	1907037	24859	40
Euro OTC	Aspartato de ornitina	2201011	25959	40
Euro OTC	Aspartato de ornitina	2201011	25959SI	40
Euro OTC	Aspartato de ornitina	2301047	26592SI†	20
Euro OTC	Aspartato de ornitina	2307023	26877SI†	20

- 201 844 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Aspartato de ornitina*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Aspartato de ornitina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Aspartato de ornitina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	425	0	152 537
Type B	0	240	0	201 844
Type C	0	0	0	236 067

The substance/substance group *Aspartato de ornitina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5882 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21694	21694	0,00	134,01
21710	21710	0,00	112,60
22599	21694	6,72	134,76
22600	21710	11,74	110,88
22924	22924	0,00	119,50
23198	21694	11,02	138,74
23864	23864	0,00	97,99
26592	26592	0,00	115,12
26877	26877	0,00	114,77
27404	27404	0,00	98,77

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Aspartato monobásico de magnésio tetra-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20812-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Aspartato monobásico de magnésio tetra-hidratado; Magnesii aspartas tetrahydricus

Special notes

When selecting the *Aspartato monobásico de magnésio tetra-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Aspartato monobásico de magnésio tetra-hidratado	7	6	10

Second-stage model

For differentiation of the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	73,96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Aspartato monobásico de m…	1204014-01	20812	40	1404588
Euro OTC	Aspartato monobásico de m…	1306045-01	21749	60	20130708
Euro OTC	Aspartato monobásico de m…	1605031	22682	40	20160617*
Euro OTC	Aspartato monobásico de m…	1901036	24488	40	20190227*
Euro OTC	Aspartato monobásico de m…	1906029	24773	40	20190712*
Euro OTC	Aspartato monobásico de m…	2002039	25125	40	20200331*
Euro OTC	Aspartato monobásico de m…	2303004	26645	40	20230315*
Euro OTC	Aspartato monobásico de m…	2303004	26645SI	20	20230315*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 9 reference samples from the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Aspartato monobásico de m…	1707010	23552	40
Euro OTC	Aspartato monobásico de m…	1806011	24156	40
Euro OTC	Aspartato monobásico de m…	2007041	25344	40
Euro OTC	Aspartato monobásico de m…	2101039	25737	40
Euro OTC	Aspartato monobásico de m…	2207024	26273	40
Euro OTC	Aspartato monobásico de m…	2407011	27340	40
Euro OTC	Aspartato monobásico de m…	1707010	23608	40
Euro OTC	Aspartato monobásico de m…	2207024	26273SI	20
Euro OTC	Aspartato monobásico de m…	2407011	27340SI	20

- 201 764 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 4 *Apo-Ident* customers from 10 batches from the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Aspartato monobásico de m…	2303004-01	1
Euro OTC	Aspartato monobásico de m…	1605031-01	1
Euro OTC	Aspartato monobásico de m…	1806011-01	1
Euro OTC	Aspartato monobásico de m…	1901036-02	1
Euro OTC	Aspartato monobásico de m…	2002039-01	3
Euro OTC	Aspartato monobásico de m…	2007041-01	3
Euro OTC	Aspartato monobásico de m…	210039-01	1
Euro OTC	Aspartato monobásico de m…	2101039-01	5
Euro OTC	Aspartato monobásico de m…	3068139	1
Euro OTC	Aspartato monobásico de m…	3843631-1	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 248 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Aspartato monobásico de magnésio tetra-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Aspartato monobásico de magnésio tetra-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	320	0	201 764
Type C	0	18	0	236 049

The substance/substance group *Aspartato monobásico de magnésio tetra-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20812	20812	0,00	147,41
21749	20812	11,69	149,05
22682	22682	0,00	145,28
24488	24488	0,00	145,18
24773	24773	0,00	146,10
25125	25125	0,00	149,66
26645	26645	0,00	149,70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Azul patente V**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20469-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Azul patente V

Special notes

When selecting the *Azul patente V* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Azul patente V	6	2	15

Second-stage model

For differentiation of the substance/substance group *Azul patente V* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Azul patente V* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	55,34	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Azul patente V* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Azul patente V*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Azul patente V	12364206	21384	40	1508043
Caelo	Azul patente V	12364206	21385	40	20130110
Caelo	Azul patente V	13351803	21695	60	20131114
Caelo	Azul patente V	13351807	22387	40	1702362
Caelo	Azul patente V	190746	24731	40	20190425*
Caelo	Azul patente V	20000907	25212	40	20200604*
Caelo	Azul patente V	21002827	26118	40	20210923*
Caelo	Azul patente V	21002827	26118SI	20	20210923*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Azul patente V*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Azul patente V*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Azul patente V	16306902	23214	40
Caelo	Azul patente V	22002332	26354	40
Caelo	Azul patente V	16306902	23215	40
Caelo	Azul patente V	22002332	26354SI	20

- 201 944 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 67 spectra from 58 *Apo-Ident* customers from 18 batches from the substance/substance group *Azul patente V*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Azul patente V	22002332005	2
Bombastus	Azul patente V	11305302	1
Bombastus	Azul patente V	17034204	1
Caelo	Azul patente V	11305302	1
Caelo	Azul patente V	11305303	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Azul patente V	12364202	1
Caelo	Azul patente V	12364206	4
Caelo	Azul patente V	13351803	1
Caelo	Azul patente V	13351807	5
Caelo	Azul patente V	13351808	1
Caelo	Azul patente V	150602	1
Caelo	Azul patente V	15060204	2
Caelo	Azul patente V	16306904	4
Caelo	Azul patente V	17034204	8
Caelo	Azul patente V	17034207	6
Caelo	Azul patente V	17034210	4
Caelo	Azul patente V	19074603	8
Caelo	Azul patente V	20000907006	3
Caelo	Azul patente V	2759	1
Caelo	Azul patente V	P-15051823/17034204	1
Caesar & Loretz GmbH/Gehe	Azul patente V	19074603	1
Caesar & Loretz GmbH/Gehe	Azul patente V	20000907006	1
Caesar & Loretz GmbH	Azul patente V	17034207	1
Caesar & Loretz GmbH	Azul patente V	19074603	1
Caesar & Loretz GmbH	Azul patente V	20000907006	3
Euro OTC	Azul patente V	17034210	1
GEHE	Azul patente V	17034207	1

- 236 000 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Azul patente V* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Azul patente V* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	140	0	201 944
Type C	0	67	0	236 000

The substance/substance group *Azul patente V* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.0448 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21384	21384	0,00	150,30
21385	21384	3,70	148,79
21695	22387	6,43	132,68
22387	22387	0,00	136,11
24731	24731	0,00	92,77
25212	25212	0,00	86,82
26118	26118	0,00	99,83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bacitracina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20851-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bacitracina; Bacitracinum

Special notes

When selecting the *Bacitracina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bacitracina	6	4	102

Second-stage model

For differentiation of the substance/substance group *Bacitracina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bacitracina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	36,39	22,89
Sulfato de colistina	59,82	19,45
⋮	⋮	⋮
Cianocobalamina	>50	55,17
Anfotericina B	>50	55,60
Pantotenato de cálcio	>50	57,41
Metilcobalamina	>50	71,19
Triancinolona	>50	72,36
Vitamina E acetato pó 50%	>50	73,74
Nistatina	>50	74,11
Estriol	>50	78,92
Gelatina, branca	>50	78,94
Estradiol hemi-hidratado	>50	104,46
Riboflavina	>50	130,60
Levedura de selênio	>50	155,60
Glicerofosfato de cálcio	>50	187,25
Carmelose sódica	>50	213,34
Bromidrato de hioscina	>50	222,17
SyrSpend® SF Alka	>50	260,96
Tosilcloramida sódica	>50	267,42
Amido de arroz	>50	344,40
Ácido oxálico	>50	364,87
Amido de milho	>50	441,99
SyrSpend® SF pH4 neo	>50	451,03
Goma arábica, dispersão seca	>50	472,58
SyrSpend® SF pH4	>50	543,47
Maltodextrina	>50	612,74
Amido de trigo	>50	644,50
Fécula de batata	>50	680,90
Frutose	>50	720,57

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bacitracina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bacitracina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bacitracina	13A-03-N11	20851	40	1401189
Fagron	Bacitracina	14A21-B09-292909	21657	60	1511741
Fagron	Bacitracina	14E23-B03-296243	21686	60	1503715
Fagron	Bacitracina	15C12-B06-309185	21898	60	20150324
Fagron	Bacitracina	15C12-B06-309185	21986	60	9466
Fagron	Bacitracina	16B17-B03-322939	22739	40	20160421
Fagron	Bacitracina	20E-14-F01-373034	25374	40	20200828

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 7 reference samples from the substance/substance group *Bacitracina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 602 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Bacitracina*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Bacitracina	16I12-B03-334194	23531	40
Fagron	Bacitracina	17L11-B02-343685	23933	40
Fagron	Bacitracina	18K14-B04-358690	24815	40
Fagron	Bacitracina	23A04-B07-225071	26603	40
Fagron	Bacitracina	23A04-B07-225071	26603SI	20

- 201 904 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 314 spectra from 176 *Apo-Ident* customers from 113 batches from the substance/substance group *Bacitracina*.

- Among them are spectra of independent samples from 102 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bacitracina	21H03-B04	1
	Bacitracina	21H03-B04-220048	1
	Bacitracina	23A04-B07-225070	4
	Bacitracina	B0722507000	1
18K14-B04-367499	Bacitracina	Fagron	1
AHD	Bacitracina	17L11-B02-344244	1
Bombastus	Bacitracina	17L11-B02-354799	1
Caelo	Bacitracina	14A21-B09-292908	1
Caelo	Bacitracina	14E23-B03-296243	2
Caelo	Bacitracina	15080605	1
Caelo	Bacitracina	15C12-B06-317782	1
Caelo	Bacitracina	16/12-B03	1
Caelo	Bacitracina	16B17-B03	1
Caelo	Bacitracina	16I12-B03-331152	1
Caelo	Bacitracina	17L11-B02-343685	1
Caelo	Bacitracina	17L11-B02-354799	1
Caelo	Bacitracina	17L11-B02-357635	1
Caelo	Bacitracina	C2280092	1
Caelo	Bacitracina	F01-3732508	2
Euro OTC	Bacitracina	17L11-B02-348461	1
fag	Bacitracina	17L11-B02-346531	1
Fagraon	Bacitracina	14E23-B03-303424	1
Fagron	Bacitracina		1
Fagron	Bacitracina	11J17-N01	2
Fagron	Bacitracina	12G12-N17	1
Fagron	Bacitracina	13A03-N11	1
Fagron	Bacitracina	13B25-B01	1
Fagron	Bacitracina	13C13-N10	1
Fagron	Bacitracina	13D26-N08	1
Fagron	Bacitracina	14A21-B09	2
Fagron	Bacitracina	14A21-B09-290643	2
Fagron	Bacitracina	14A21-B09-290645	2
Fagron	Bacitracina	14A21-B09-292908	2
Fagron	Bacitracina	14E23-B03	3
Fagron	Bacitracina	14e23-b03-296243	1
Fagron	Bacitracina	14E23-B03-296243	6
Fagron	Bacitracina	14E23-B03-296245	2
Fagron	Bacitracina	14E23B03303424	1
Fagron	Bacitracina	14E23B03-303424	1
Fagron	Bacitracina	14E23-B03-303424	3
Fagron	Bacitracina	14E23-B03-333424	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bacitracina	15C12-B06	1
Fagron	Bacitracina	15C12-B06-309185	1
Fagron	Bacitracina	15C12-B06-317782	1
Fagron	Bacitracina	16/12-B03-329401	3
Fagron	Bacitracina	16/12-B03-331152	1
Fagron	Bacitracina	16/12-B03-334052	3
Fagron	Bacitracina	16/12-B03-334701	1
Fagron	Bacitracina	16/12B03335331	1
Fagron	Bacitracina	16/12-B03-335331	1
Fagron	Bacitracina	1612-B033-334052	1
Fagron	Bacitracina	16B17-B03	2
Fagron	Bacitracina	16B17-B03-321315	1
Fagron	Bacitracina	16b17-b03-322891	1
Fagron	Bacitracina	16B17-b03-322891	1
Fagron	Bacitracina	16B17-B03-322891	10
Fagron	Bacitracina	16b17-b03-322939	1
Fagron	Bacitracina	16B17-B03-322939	1
Fagron	Bacitracina	16B17-B03-323876	1
Fagron	Bacitracina	16B17b03325856	1
Fagron	Bacitracina	16B17B03325856	1
Fagron	Bacitracina	16B17-B03-325856	1
Fagron	Bacitracina	16I12-B03	3
Fagron	Bacitracina	16I12-B03-329401	1
Fagron	Bacitracina	16i12-b03-334052	1
Fagron	Bacitracina	16I12-B03-334052	5
Fagron	Bacitracina	16I12-B03-335331	3
Fagron	Bacitracina	17L11-802	1
Fagron	Bacitracina	17L11-B02	9
Fagron	Bacitracina	17L11-B02_357635	1
Fagron	Bacitracina	17L11-B02-343685	14
Fagron	Bacitracina	17L11-B02-343686	1
Fagron	Bacitracina	17L11-B02-346531	3
Fagron	Bacitracina	17L11-B02-346961	2
Fagron	Bacitracina	17L11B02348461	1
Fagron	Bacitracina	17L11-B02-348461	11
Fagron	Bacitracina	17L11-B02-35400	1
Fagron	Bacitracina	17L11-B02-354799	8
Fagron	Bacitracina	17L11B02357635	1
Fagron	Bacitracina	17L11-B02-357635	7
Fagron	Bacitracina	17L11-B02-357980	1
Fagron	Bacitracina	18K14-B04	10
Fagron	Bacitracina	18k14-B04-358690	1
Fagron	Bacitracina	18K14-B04-358690	17
Fagron	Bacitracina	18K14-B04-358692	1
Fagron	Bacitracina	18K14B04363373	1
Fagron	Bacitracina	18K14-B04363373	1
Fagron	Bacitracina	18K14-B04-363373	6
Fagron	Bacitracina	18K14-B04-367499	3
Fagron	Bacitracina	18K14-B04-368113	1
Fagron	Bacitracina	18K14-B0463373	1
Fagron	Bacitracina	18K14-B04-363374	1
Fagron	Bacitracina	20E14-F01	5
Fagron	Bacitracina	20E14-F01-373033	1
Fagron	Bacitracina	20E14-F01-373258	6
Fagron	Bacitracina	20K20-F02-376064	1
Fagron	Bacitracina	211531	1
Fagron	Bacitracina	21H03_B04_220048	1
Fagron	Bacitracina	21H03-804-216119	1
Fagron	Bacitracina	21H03-B04-216119	3
Fagron	Bacitracina	21H03-B04-216120	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bacitracina	21H03-B04-220048	3
Fagron	Bacitracina	28051509	1
Fagron	Bacitracina	2917M-03314	1
Fagron	Bacitracina	31071503	1
Fagron	Bacitracina	358690	1
Fagron	Bacitracina	B04-3633703	2
Fagron	Bacitracina	B04-3633704	2
Fagron	Bacitracina	B04-3674909	2
Fagron	Bacitracina	B04-3681103	1
Fagron	Bacitracina	C2208111	2
Fagron	Bacitracina	C2280017	3
Fagron	Bacitracina	C2280054	1
Fagron	Bacitracina	C2280065	3
Fagron	Bacitracina	C2280092	3
Fagron	Bacitracina	C2280111	8
Fagron	Bacitracina	C2280138	3
Fagron	Bacitracina	F01-3730303	2
Fagron	Bacitracina	F01-3732508	5
Fargon - Alliance He...	Bacitracina	21H03-B04-216119	1
Fargon/Gehe	Bacitracina	C2280092	1
Fargon/Phönix	Bacitracina	15C12-B06-312975	1
Fargon/Phönix	Bacitracina	18K14-B04	1
Fargon	Bacitracina	16B17-B03-325856	2
fargon	Bacitracina	17L11-B02-357635	1
Fargron	Bacitracina	16/14-b03-334701	1
Fischar/ Now	Bacitracina	18K14-B04-367499	2
Fragon/ Gehe	Bacitracina	17L11-B02	1
Fragon/Phönix	Bacitracina	16/12-B03-329401	1
Gehe	Bacitracina	16/12-B03-331185	1
Gehe	Bacitracina	16B17-B03-322891	1
Gehe	Bacitracina	17L11-B02-343685	1
Gehe	Bacitracina	17L11-B02-346531	1
Gehe	Bacitracina	17L11-B02-348461	1
gehe	Bacitracina	21H03-B04-216120	2
Gehe	Bacitracina	C2280065	1
Geibo/ Fargron	Bacitracina	16B17-B03-322891	1
Geilenkirchen	Bacitracina	16/12-B03-329401	1
Kehr	Bacitracina	16B17-B03-322891	1
Noweda	Bacitracina	17L11-B02-346961	2
Noweda	Bacitracina	17L11-B02-354800	3
Noweda	Bacitracina	18K14-B04-363373	1
Phönix Gotha	Bacitracina	C2280010	1
Phönix	Bacitracina	c2280065	1
Sanacorp	Bacitracina	18K14-B04	1
Sanacorp	Bacitracina	20E14-F01-373258	1
Sanacorp	Bacitracina	21H03-B04-220048	1
Sanacorp	Bacitracina	21h03-b04-220074	1
sanacorp	Bacitracina	2280111	1
Sanacorp	Bacitracina	23A04-B07-225070	1

- 235 753 spectra from 1515 *Apo-Ident* customers from a total of 49 147 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Bacitracina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bacitracina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	180	0	201 904
Type C	0	312	2	235 753

The substance/substance group *Bacitracina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	99.3631 % (> 98.4076 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20851	20851	0,00	61,20
21657	21657	0,00	64,71
21686	21686	0,00	68,79
21898	21986	12,70	69,78
21986	21986	0,00	67,98
22739	20851	14,92	66,15
25374	21686	21,82	77,09

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Baclofeno**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	23375-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Baclofeno; Baclofenum

Special notes

When selecting the *Baclofeno* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Baclofeno	6	3	8

Second-stage model

For differentiation of the substance/substance group *Baclofeno* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Baclofeno* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	128,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Baclofeno* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Baclofeno*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Baclofeno	21D09-F05-377817	25716	50	20210503
Fagron	Baclofeno	21K12-B21-221120	26177	40	20211222
Fagron	Baclofeno	21K12-B21-221120	26177SI	20	20211222
Fagron	Baclofeno	22K19-B06-225423	26463	40	20221201
Fagron	Baclofeno	23K24-B02-234668	27046	40	20231129
Fagron	Baclofeno	23K24-B02-234668	27046SI	20	20231129
Fagron	Baclofeno	24E21-B01-238856	27300	40	20240613
Inresa	Baclofeno	206031617/09062017	23376	40	AR-17-FG-018577-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 290 spectra of 8 reference samples from the substance/substance group *Baclofeno*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 672 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Baclofeno*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Baclofeno	18I28-B02-356294	24444	40
Fagron	Baclofeno	20J01-F06-374476	25489	40
Fagron	Baclofeno	23G19-B03-230417	26912	40
Fagron	Baclofeno	23G19-B03-230417	26912SI	20

- 201 944 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 37 spectra from 30 *Apo-Ident* customers from 13 batches from the substance/substance group *Baclofeno*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Baclofeno		1
	Baclofeno	1234567890	1
	Baclofeno	201062126	1
	Baclofeno	201072217	2
	Baclofeno	21K12-B21-221120	2
	Baclofeno	22K19-B06-225423	6
	Baclofeno	23K24-B02-234668	2
Alliance Healthcare	Baclofeno	23K24-B02-234668	1
Fagron	Baclofeno	202022126	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Baclofeno	21D09-F05	3
Fagron	Baclofeno	21d09-f05-377817	1
Fagron	Baclofeno	21D09-F05377817	1
Fagron	Baclofeno	21D09-F05-377817	12
Gehe	Baclofeno	23G19-B03-230417	1
Pharmac. works Polph…	Baclofeno	201062126	1

- 236 030 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Baclofeno* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Baclofeno* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	140	0	201 944
Type C	0	37	0	236 030

The substance/substance group *Baclofeno* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 83.7838 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23376	23376	0,00	209,82
25716	23376	7,86	217,41
26177	23376	10,09	216,81
26463	23376	16,03	204,59
27046	23376	12,77	216,79
27300	23376	8,01	214,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Barbital sódico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20309-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Barbital sódico; Barbitalum natricum

Special notes

When selecting the *Barbital sódico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Barbital sódico	2	1	1

Second-stage model

For differentiation of the substance/substance group *Barbital sódico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Barbital sódico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	96,46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Barbital sódico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Barbital sódico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Barbital sódico	12F27-N02	21136	40	0814I-07775
Fagron	Barbital sódico	12F27-N02	21136SI	60	0814I-07775
Fagron	Barbital sódico	14K14-B04-303353	22429	60	1516I-07775
Fagron	Barbital sódico	14K14-B04-303353	22429SI	60	1516I-07775

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 4 reference samples from the substance/substance group *Barbital sódico*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 742 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Barbital sódico*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Barbital sódico	15L07-B02-324539	23463	40
Fagron	Barbital sódico	15L07-B02-324539	23463SI	40

- 202 004 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Barbital sódico*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Barbital sódico	15L07-B02	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Barbital sódico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

relevant spectra of the various substances were compared with *Barbital sódico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	80	0	202 004
Type C	0	1	0	236 066

The substance/substance group *Barbital sódico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21136	21136	0,00	154,13
22429	22429	0,00	158,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Benzoato de estradiol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20098-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Benzoato de estradiol; Estradioli benzoas

Special notes

When selecting the *Benzoato de estradiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Benzoato de estradiol	7	5	133

Second-stage model

For differentiation of the substance/substance group *Benzoato de estradiol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Benzoato de estradiol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	152,15	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Benzoato de estradiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Benzoato de estradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzoato de estradiol	15078608	23218	40	20150415
Caelo	Benzoato de estradiol	181444	24254	40	20180614*
Caelo	Benzoato de estradiol	21004177006	26314	40	20220112
Caelo	Benzoato de estradiol	21004177006	26314SI	40	20220112
Euro OTC	Benzoato de estradiol	1301006-02	21290	40	1507405
Euro OTC	Benzoato de estradiol	1507009	21869	60	0000010566
Euro OTC	Benzoato de estradiol	1507009	21869SI	60	0000010566
Fagron	Benzoato de estradiol	12H02-N02	20889	40	20120817
Fagron	Benzoato de estradiol	12H02-N02	20889SI	60	20120817
Fagron	Benzoato de estradiol	14B20-B02	21257	40	20140327
Fagron	Benzoato de estradiol	14B20-B02	21257SI	60	20140327

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 520 spectra of 11 reference samples from the substance/substance group *Benzoato de estradiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 442 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 11 reference samples from the substance/substance group *Benzoato de estradiol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzoato de estradiol	13277607	21324	40
Euro OTC	Benzoato de estradiol	1611004	22873	40
Euro OTC	Benzoato de estradiol	1412033	24139	40
Euro OTC	Benzoato de estradiol	2001032	25113	40
Fagron	Benzoato de estradiol	24B26-B06-228380	27184	40
Caelo	Benzoato de estradiol	15078608	23218SI†	40
Caelo	Benzoato de estradiol	181444	24254SI†	40
Euro OTC	Benzoato de estradiol	1611004	22873SI	40
Euro OTC	Benzoato de estradiol	1412033	24139SI	40
Euro OTC	Benzoato de estradiol	2001032	25113SI	40
Fagron	Benzoato de estradiol	24B26-B06-228380	27184SI	40

- 201 644 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 884 spectra from 547 *Apo-Ident* customers from 142 batches from the substance/substance group *Benzoato de estradiol*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 132 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Benzoato de estradiol	2001032	1
	Benzoato de estradiol	2001032-03	2
	Benzoato de estradiol	21004177005	1
	Benzoato de estradiol	2300012002	1
	Benzoato de estradiol	23000121002	4
	Benzoato de estradiol	23000121003	7
	Benzoato de estradiol	23000121005	1
	Benzoato de estradiol	3919E-01946	1
A.H. 07.06.13 ek: 24,14EUR	Benzoato de estradiol	1201019-02	1
AHC	Benzoato de estradiol	18144408	1
AHD	Benzoato de estradiol	14B20-B02-292001	1
AHD	Benzoato de estradiol	1611004-02	1
AHD	Benzoato de estradiol	18144404	1
aliance healthcare 5...	Benzoato de estradiol	10118576	1
Alliance Healthcare	Benzoato de estradiol	1301006-01	1
apo-ident	Benzoato de estradiol	18144405	1
Bayer Pharma AG / Noweda	Benzoato de estradiol	14B20-B02	1
Bayer Pharma/Noweda	Benzoato de estradiol	14B20-B02-292001	1
Bayer-Schering	Benzoato de estradiol	1007037-03	1
Caelo	Benzoato de estradiol		4
Caelo	Benzoato de estradiol	10124909	5
Caelo	Benzoato de estradiol	10124912	1
Caelo	Benzoato de estradiol	10124915	2
Caelo	Benzoato de estradiol	10124918	2
Caelo	Benzoato de estradiol	10124919	1
Caelo	Benzoato de estradiol	10124921	1
Caelo	Benzoato de estradiol	1100417	1
Caelo	Benzoato de estradiol	111004-02	1
Caelo	Benzoato de estradiol	1149	1
Caelo	Benzoato de estradiol	1201019-02	1
Caelo	Benzoato de estradiol	12255904	10
Caelo	Benzoato de estradiol	12255905	10
Caelo	Benzoato de estradiol	1301006-02	1
Caelo	Benzoato de estradiol	13276401	6
Caelo	Benzoato de estradiol	13277602	8
Caelo	Benzoato de estradiol	13277603	2
Caelo	Benzoato de estradiol	13277605	4
Caelo	Benzoato de estradiol	13277607	3
Caelo	Benzoato de estradiol	1401001-01	1
Caelo	Benzoato de estradiol	1412033-02	1
Caelo	Benzoato de estradiol	1507009-01	1
Caelo	Benzoato de estradiol	1507806	1
Caelo	Benzoato de estradiol	15078602	8
Caelo	Benzoato de estradiol	15078603	22
Caelo	Benzoato de estradiol	15078604	21
Caelo	Benzoato de estradiol	15078606	6
Caelo	Benzoato de estradiol	15078608	16
Caelo	Benzoato de estradiol	15078609	1
Caelo	Benzoato de estradiol	150918EB	1
Caelo	Benzoato de estradiol	15C10B04305523	1
Caelo	Benzoato de estradiol	15C10-B04-305523	2
Caelo	Benzoato de estradiol	16003701	7
Caelo	Benzoato de estradiol	16003702	7
Caelo	Benzoato de estradiol	16003707	22
Caelo	Benzoato de estradiol	1611004-01	1
Caelo	Benzoato de estradiol	1611004-02	2
Caelo	Benzoato de estradiol	17357602	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Benzoato de estradiol	17357604	2
Caelo	Benzoato de estradiol	17357605	12
Caelo	Benzoato de estradiol	1814404	1
Caelo	Benzoato de estradiol	1814405	1
Caelo	Benzoato de estradiol	1814408	1
Caelo	Benzoato de estradiol	18144402	23
Caelo	Benzoato de estradiol	18144404	19
Caelo	Benzoato de estradiol	18144405	31
Caelo	Benzoato de estradiol	18144406	17
Caelo	Benzoato de estradiol	18144406P-191101-1	1
Caelo	Benzoato de estradiol	18144408	22
Caelo	Benzoato de estradiol	181444404	1
Caelo	Benzoato de estradiol	181444405	1
Caelo	Benzoato de estradiol	181444406	1
Caelo	Benzoato de estradiol	1844406	1
Caelo	Benzoato de estradiol	200000164001	2
Caelo	Benzoato de estradiol	20000164001	53
Caelo	Benzoato de estradiol	2000016401	2
Caelo	Benzoato de estradiol	2000164001	1
Caelo	Benzoato de estradiol	2001032-01	1
Caelo	Benzoato de estradiol	21000144002	1
Caelo	Benzoato de estradiol	21000145001	18
Caelo	Benzoato de estradiol	21000145003	8
Caelo	Benzoato de estradiol	21004177003	18
Caelo	Benzoato de estradiol	21004177004	4
Caelo	Benzoato de estradiol	21004177005	10
Caelo	Benzoato de estradiol	21004177006	11
Caelo	Benzoato de estradiol	21004177008	11
Caelo	Benzoato de estradiol	21121204	1
Caelo	Benzoato de estradiol	227051-08-08	1
Caelo	Benzoato de estradiol	23000121002	3
Caelo	Benzoato de estradiol	32308779	1
Caelo	Benzoato de estradiol	6091305	1
Caelo	Benzoato de estradiol	81403700	1
Caelo	Benzoato de estradiol	84303830	2
Caelo	Benzoato de estradiol	92137389	1
Caelo	Benzoato de estradiol	eucerin	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21004177003	1
Caesar & Loretz GmbH...	Benzoato de estradiol	18144404	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21004177008	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21000145003	1
Caesar & Loretz GmbH/AHD	Benzoato de estradiol	21004177006	1
Caesar & Loretz GmbH...	Benzoato de estradiol	18144404	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21000145001	1
Caesar & Loretz GmbH/Gehe	Benzoato de estradiol	18144405	1
Caesar & Loretz GmbH/GEHE	Benzoato de estradiol	18144405	1
Caesar & Loretz GmbH/GEHE	Benzoato de estradiol	18144406	1
Caesar & Loretz GmbH/Gehe	Benzoato de estradiol	20000164001	1
Caesar & Loretz GmbH/Gehe	Benzoato de estradiol	21004177004	2
Caesar & Loretz GmbH...	Benzoato de estradiol	20000164001	1
Caesar & Loretz GmbH/Kehr	Benzoato de estradiol	20000164001	1
Caesar & Loretz GmbH...	Benzoato de estradiol	18144402	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21000145001	1
Caesar & Loretz GmbH/Ph	Benzoato de estradiol	18144408	1
Caesar & Loretz GmbH...	Benzoato de estradiol	20000164001	1
Caesar & Loretz GmbH...	Benzoato de estradiol	18144404	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21004177005	1
Caesar & Loretz GmbH...	Benzoato de estradiol	21004177003	1
Caesar & Loretz GmbH	Benzoato de estradiol	17357605	4
Caesar & Loretz GmbH	Benzoato de estradiol	18144402	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Benzoato de estradiol	18144405	12
Caesar & Loretz GmbH	Benzoato de estradiol	18144406	9
Caesar & Loretz GmbH	Benzoato de estradiol	18144408	4
Caesar & Loretz GmbH	Benzoato de estradiol	20000164001	8
Caesar & Loretz GmbH	Benzoato de estradiol	21000145001	6
Caesar & Loretz GmbH	Benzoato de estradiol	21000145003	3
Caesar & Loretz GmbH	Benzoato de estradiol	21004177003	4
Caesar & Loretz GmbH	Benzoato de estradiol	21004177004	4
Caesar & Loretz GmbH	Benzoato de estradiol	21004177005	3
Caesar & Loretz GmbH	Benzoato de estradiol	21004177006	12
Caesar & Loretz GmbH	Benzoato de estradiol	21004177008	1
Caesar & Loretz GmbH	Benzoato de estradiol	23000121002	2
Caesar & Loretz	Benzoato de estradiol	17357605	1
Caesar / Gehe	Benzoato de estradiol	16003707	1
Caesar L / Sanacorp	Benzoato de estradiol	18144408	1
Caesar&Lorenz / Gehe	Benzoato de estradiol	18144405	1
Caesar&Lorenz	Benzoato de estradiol	21000145001	1
Cealo/Noweda	Benzoato de estradiol	18144405	1
Cealo	Benzoato de estradiol	15078604	1
EuRho/Sanacorp	Benzoato de estradiol	1201019-02	1
EuRho	Benzoato de estradiol	84303830	1
Euro OTC	Benzoato de estradiol	1007037-02	1
Euro OTC	Benzoato de estradiol	1201019-01	7
Euro OTC	Benzoato de estradiol	1201019-02	9
Euro OTC	Benzoato de estradiol	121019-01	1
Euro OTC	Benzoato de estradiol	130100601	1
Euro OTC	Benzoato de estradiol	1301006-01	2
Euro OTC	Benzoato de estradiol	1301006-02	11
Euro OTC	Benzoato de estradiol	14010001-01	1
Euro OTC	Benzoato de estradiol	1401001-01	10
Euro OTC	Benzoato de estradiol	140101-01	1
Euro OTC	Benzoato de estradiol	1412033-01	9
Euro OTC	Benzoato de estradiol	1412033-02	6
Euro OTC	Benzoato de estradiol	150700901	2
Euro OTC	Benzoato de estradiol	1507009-01	16
Euro OTC	Benzoato de estradiol	1507009-01I-0401016	1
Euro OTC	Benzoato de estradiol	16003707	1
Euro OTC	Benzoato de estradiol	1611004-01	11
Euro OTC	Benzoato de estradiol	161100402	2
Euro OTC	Benzoato de estradiol	1611004-02	21
Euro OTC	Benzoato de estradiol	1611004-028638831	1
Euro OTC	Benzoato de estradiol	16110047-02	1
Euro OTC	Benzoato de estradiol	16111004-01	1
Euro OTC	Benzoato de estradiol	1807161	1
Euro OTC	Benzoato de estradiol	2001032-01	15
Euro OTC	Benzoato de estradiol	2001032-02	3
Euro OTC	Benzoato de estradiol	2001032-03	2
Euro OTC	Benzoato de estradiol	21000145003	1
Euro OTC	Benzoato de estradiol	8011422	1
Euro OTC	Benzoato de estradiol	83101340	1
Euro OTC	Benzoato de estradiol	84303830	2
EURO Pharma	Benzoato de estradiol	84303830	1
Euro/Krieger	Benzoato de estradiol	1611004-02	1
Fagron	Benzoato de estradiol	11H01-N12	1
Fagron	Benzoato de estradiol	11L23-N01	2
Fagron	Benzoato de estradiol	12B08-N05	1
Fagron	Benzoato de estradiol	12D20N06	1
Fagron	Benzoato de estradiol	12H02-N02	3
Fagron	Benzoato de estradiol	12H02-N052	1
Fagron	Benzoato de estradiol	12L14-N02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Benzoato de estradiol	13/11-N01	2
Fagron	Benzoato de estradiol	13C15-B07-288645	1
Fagron	Benzoato de estradiol	13I11N01	1
Fagron	Benzoato de estradiol	13I11-N01	1
Fagron	Benzoato de estradiol	1412033-01	1
Fagron	Benzoato de estradiol	14820-B02-294949	1
Fagron	Benzoato de estradiol	14B20-B02	3
Fagron	Benzoato de estradiol	14B20-B02-2920001	1
Fagron	Benzoato de estradiol	14B20-B02-292001	6
Fagron	Benzoato de estradiol	14b20-b02-294949	1
Fagron	Benzoato de estradiol	14B20-B02-294949	3
Fagron	Benzoato de estradiol	15c10-b04-305523	1
Fagron	Benzoato de estradiol	15C10-B04-305523	6
Fagron	Benzoato de estradiol	15E08-B08	1
Fagron	Benzoato de estradiol	15E08-B08-311705	13
Fagron	Benzoato de estradiol	17357602	1
Fagron	Benzoato de estradiol	17L01-B05-3434714	1
Fagron	Benzoato de estradiol	17L01B05343714	1
Fagron	Benzoato de estradiol	17L01-B05-343714	4
Fagron	Benzoato de estradiol	17L01-B05-348601	1
Fagron	Benzoato de estradiol	2001032-01	1
Fagron	Benzoato de estradiol	20D16-F08-370349	1
Fagron	Benzoato de estradiol	2x12L14-N02	1
Fagron	Benzoato de estradiol	81403680	1
Fagron	Benzoato de estradiol	81403690	3
Fagron	Benzoato de estradiol	83101340	2
Fagron	Benzoato de estradiol	84303830	1
Fagron	Benzoato de estradiol	84303840	1
Fargon/AHD	Benzoato de estradiol	15E08-B08-311705	2
Fiebig	Benzoato de estradiol	20000164001	1
Finze	Benzoato de estradiol	1003040-01	2
Gehe	Benzoato de estradiol	11L23-N01	1
Gehe	Benzoato de estradiol	15078606	1
GEHE	Benzoato de estradiol	15078609	1
Gehe	Benzoato de estradiol	17L01-B05-343714	1
Gehe	Benzoato de estradiol	18144405	2
Gehe	Benzoato de estradiol	18144408	1
Gehe	Benzoato de estradiol	20000164001	1
Gehe	Benzoato de estradiol	2001032-02	1
Gehe	Benzoato de estradiol	21004177005	1
Gehe	Benzoato de estradiol	23000121002	1
GUMO	Benzoato de estradiol	21000145001	1
Jenne/Caesar & Loret…	Benzoato de estradiol	21004177004	1
Kehr	Benzoato de estradiol	18144404	1
Kehr	Benzoato de estradiol	23000121003	1
Klenk	Benzoato de estradiol	8(18144402)	1
Krieger	Benzoato de estradiol	3401	1
Nachprüfung	Benzoato de estradiol	123456	1
Noweda	Benzoato de estradiol	13277603	1
Noweda	Benzoato de estradiol	15078608	1
Noweda	Benzoato de estradiol	18144402	1
Noweda	Benzoato de estradiol	2001032-01	1
Noweda	Benzoato de estradiol	21000145001	2
Noweda	Benzoato de estradiol	21004177003	1
Noweda	Benzoato de estradiol	21004177004	1
Phoenix 1.10.2018	Benzoato de estradiol	17357602	1
Phoenix WE:20.11.17 …	Benzoato de estradiol	16003702	1
Phoenix/Cealo	Benzoato de estradiol	1611004-01	1
Phoenix	Benzoato de estradiol	15078608	1
Phoenix	Benzoato de estradiol	18144402	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Benzoato de estradiol	20d16-f08-373007	1
Phoenix	Benzoato de estradiol	8638831	1
phönix	Benzoato de estradiol	14B20-B02-294949	1
Phönix	Benzoato de estradiol	16003707	2
phönix	Benzoato de estradiol	21004177004	1
Sanacorp 04.07.19 Ek…	Benzoato de estradiol	18144404	1
Sanacorp	Benzoato de estradiol	10/AKD24	1
sanacorp	Benzoato de estradiol	15078604	1
Sanacorp	Benzoato de estradiol	16003707	1
Sanacorp	Benzoato de estradiol	17L01-B05	2
Sanacorp	Benzoato de estradiol	17L01-B05-343714	1
Sanacorp	Benzoato de estradiol	1814402	1
Sanacorp	Benzoato de estradiol	21004177005	1
Sanacorp	Benzoato de estradiol	23000121002	2
Valdepharm/Phoenix	Benzoato de estradiol	ESB002-3E	1
VDl 16.10.14 12,70 euro	Benzoato de estradiol		1
VDL	Benzoato de estradiol	1507009-01	1
WE:Phönix 21.09.2012	Benzoato de estradiol	12B08-N05	1

- 235 183 spectra from 1515 *Apo-Ident* customers from a total of 49 120 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Benzoato de estradiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzoato de estradiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	440	0	201 644
Type C	0	873	11	235 183

The substance/substance group *Benzoato de estradiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	98.7557 % (> 98.4163 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20889	21290	10,50	215,63
21257	21290	4,39	213,45
21290	21290	0,00	213,66
21869	21869	0,00	217,11
23218	21869	10,39	216,26
24254	24254	0,00	216,07
26314	21869	12,41	216,29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Benzoato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006331-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Benzoato de sódio; Natrii benzoas

Special notes

When selecting the *Benzoato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Benzoato de sódio	11	17	186

Second-stage model

For differentiation of the substance/substance group *Benzoato de sódio* the following second-stage model is used:

- Submodelo 18

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Benzoato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Difenilciclopropenona	53,35	16,56

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Benzoato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Benzoato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzoato de sódio	11267016	20752	40	20110923
Caelo	Benzoato de sódio	13178619	21607	60	20130624
Euro OTC	Benzoato de sódio	1409040-01	21713	60	20141021
Euro OTC	Benzoato de sódio	1506019	21825	60	20150623*
Euro OTC	Benzoato de sódio	1510044	22236	60	20151109*
Euro OTC	Benzoato de sódio	1602020	22363	60	20160225*
Euro OTC	Benzoato de sódio	1610037	22867	40	20161202*
Euro OTC	Benzoato de sódio	1701045	22997	40	20170207*
Euro OTC	Benzoato de sódio	1711019	23900	40	20171205*
Euro OTC	Benzoato de sódio	2001018	25081	40	20200205*
Euro OTC	Benzoato de sódio	2009005	25379	40	20201001*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 540 spectra of 11 reference samples from the substance/substance group *Benzoato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 422 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 790 spectra of 21 reference samples from the substance/substance group *Benzoato de sódio*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzoato de sódio	161371	22474	60
Caelo	Benzoato de sódio	170558	23283	40
Caelo	Benzoato de sódio	173530	23784	40
Caelo	Benzoato de sódio	190541	24544	40
Caelo	Benzoato de sódio	21001722	25805	50
Caelo	Benzoato de sódio	22001421	26253	40
Caelo	Benzoato de sódio	24001874	27336	40
Euro OTC	Benzoato de sódio	1607005	22670	40
Euro OTC	Benzoato de sódio	1707024	23613	40
Euro OTC	Benzoato de sódio	1803034	24068	40
Euro OTC	Benzoato de sódio	1809005	24301	40
Euro OTC	Benzoato de sódio	1901043	24481	40
Euro OTC	Benzoato de sódio	2109016	25893	50
Euro OTC	Benzoato de sódio	2207025	26269	40
Euro OTC	Benzoato de sódio	2302017	26583	40
Euro OTC	Benzoato de sódio	2308011	26908	40
Fagron	Benzoato de sódio	15B16-B07-308570	22895	40
Caelo	Benzoato de sódio	22001421	26253SI	20
Euro OTC	Benzoato de sódio	2109016	25893SI	10
Euro OTC	Benzoato de sódio	2207025	26269SI	20
Euro OTC	Benzoato de sódio	2302017	26583SI	20

- 201 294 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 936 spectra from 573 *Apo-Ident* customers from 194 batches from the substance/substance group *Benzoato de sódio*.
- Among them are spectra of independent samples from 186 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Benzoato de sódio	2009005	1
	Benzoato de sódio	2109016-01	1
	Benzoato de sódio	22001421002	3
	Benzoato de sódio	22001421009	2
	Benzoato de sódio	22001421011	1
	Benzoato de sódio	22001421014	4
	Benzoato de sódio	22001421021	2
	Benzoato de sódio	2200142104	1
	Benzoato de sódio	2207025-01	1
	Benzoato de sódio	2308011-01	4
	Benzoato de sódio	2308011-02	2
AHD	Benzoato de sódio	1711019-01	3
AHD	Benzoato de sódio	17137606	1
AHD	Benzoato de sódio	192296011	1
AHD	Benzoato de sódio	2308011-02	1
Alliance Healthcare	Benzoato de sódio	1304024-01	1
Alliance Healthcare	Benzoato de sódio	2207025-01	1
Alliance/EurRho	Benzoato de sódio	2009005-01	1
Alliance	Benzoato de sódio	2009005-01	1
Anzag	Benzoato de sódio	20003762002	1
Anzag	Benzoato de sódio	20003762010	3
Anzag	Benzoato de sódio	21001722009	2
Bombastus	Benzoato de sódio	1404011-01	1
Bombastus	Benzoato de sódio	17055805	1
Bombastus	Benzoato de sódio	17353011	1
Caela/Phoenix	Benzoato de sódio	19054114	2
Caelo	Benzoato de sódio		1
Caelo	Benzoato de sódio	10003762015	1
Caelo	Benzoato de sódio	10544104	1
Caelo	Benzoato de sódio	11267016	1
Caelo	Benzoato de sódio	11346109	3
Caelo	Benzoato de sódio	1209018-0	1
Caelo	Benzoato de sódio	12158401	1
Caelo	Benzoato de sódio	12158418	1
Caelo	Benzoato de sódio	12158419	4
Caelo	Benzoato de sódio	12158424	1
Caelo	Benzoato de sódio	12158439	4
Caelo	Benzoato de sódio	12J23-N05	1
Caelo	Benzoato de sódio	13178603	2
Caelo	Benzoato de sódio	13178605	3
Caelo	Benzoato de sódio	13178613	1
Caelo	Benzoato de sódio	13178619	2
Caelo	Benzoato de sódio	13178627	1
Caelo	Benzoato de sódio	13178635	5
Caelo	Benzoato de sódio	13178647	2
Caelo	Benzoato de sódio	13H01-N02	1
Caelo	Benzoato de sódio	14166714	1
Caelo	Benzoato de sódio	14328702	1
Caelo	Benzoato de sódio	1503022-01	1
Caelo	Benzoato de sódio	15044102	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Benzoato de sódio	15044104	9
Caelo	Benzoato de sódio	1506019-01	1
Caelo	Benzoato de sódio	151208NB	1
Caelo	Benzoato de sódio	15135001	7
Caelo	Benzoato de sódio	15363401	12
Caelo	Benzoato de sódio	15363409	3
Caelo	Benzoato de sódio	15363413	2
Caelo	Benzoato de sódio	15363414	1
Caelo	Benzoato de sódio	15363424	11
Caelo	Benzoato de sódio	1610037-01	1
Caelo	Benzoato de sódio	161371	1
Caelo	Benzoato de sódio	16137103	12
Caelo	Benzoato de sódio	16137104	2
Caelo	Benzoato de sódio	16137112	6
Caelo	Benzoato de sódio	16137118	9
Caelo	Benzoato de sódio	17055801	5
Caelo	Benzoato de sódio	17055805	6
Caelo	Benzoato de sódio	17055806	1
Caelo	Benzoato de sódio	17061306	1
Caelo	Benzoato de sódio	17137603	1
Caelo	Benzoato de sódio	17137604	3
Caelo	Benzoato de sódio	17137606	18
Caelo	Benzoato de sódio	17137607	1
Caelo	Benzoato de sódio	17137609	1
Caelo	Benzoato de sódio	1735011	2
Caelo	Benzoato de sódio	17353001	22
Caelo	Benzoato de sódio	17353002	1
Caelo	Benzoato de sódio	17353006	2
Caelo	Benzoato de sódio	17353011	12
Caelo	Benzoato de sódio	18055805	1
Caelo	Benzoato de sódio	18161201	17
Caelo	Benzoato de sódio	18161202	1
Caelo	Benzoato de sódio	18161209	1
Caelo	Benzoato de sódio	18161211	22
Caelo	Benzoato de sódio	18161214	1
Caelo	Benzoato de sódio	1827	1
Caelo	Benzoato de sódio	1901043-02	1
Caelo	Benzoato de sódio	19054104	10
Caelo	Benzoato de sódio	19054105	4
Caelo	Benzoato de sódio	19054106	1
Caelo	Benzoato de sódio	19054114	20
Caelo	Benzoato de sódio	19091801	1
Caelo	Benzoato de sódio	191031709	1
Caelo	Benzoato de sódio	192296003	27
Caelo	Benzoato de sódio	192296004	1
Caelo	Benzoato de sódio	192296011	10
Caelo	Benzoato de sódio	192296015	12
Caelo	Benzoato de sódio	192296016	7
Caelo	Benzoato de sódio	20001291001	2
Caelo	Benzoato de sódio	20001291005	7
Caelo	Benzoato de sódio	2000376007	1
Caelo	Benzoato de sódio	2000376009	1
Caelo	Benzoato de sódio	20003762003	12
Caelo	Benzoato de sódio	20003762007	10
Caelo	Benzoato de sódio	20003762009	30
Caelo	Benzoato de sódio	20003762010	1
Caelo	Benzoato de sódio	20003762013	3
Caelo	Benzoato de sódio	20003762015	4
Caelo	Benzoato de sódio	20003792010	1
Caelo	Benzoato de sódio	2001291001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Benzoato de sódio	210014722004	1
Caelo	Benzoato de sódio	21001722003	9
Caelo	Benzoato de sódio	21001722006	11
Caelo	Benzoato de sódio	21001722008	20
Caelo	Benzoato de sódio	21001722020	4
Caelo	Benzoato de sódio	2100172203	2
Caelo	Benzoato de sódio	2100172206	1
Caelo	Benzoato de sódio	2109016-01	1
Caelo	Benzoato de sódio	2200142002	1
Caelo	Benzoato de sódio	22001421002	13
Caelo	Benzoato de sódio	22001421009	2
Caelo	Benzoato de sódio	22001421014	3
Caelo	Benzoato de sódio	2215Q-01891	1
Caelo	Benzoato de sódio	24021501	1
Caelo	Benzoato de sódio	3037647	1
Caelo	Benzoato de sódio	3918M-01891	1
Caelo	Benzoato de sódio	4315A-01891	1
Caelo	Benzoato de sódio	5117A-01891	1
Caelo	Benzoato de sódio	5211I-01891	1
Caelo	Benzoato de sódio	91443209	2
Caelo	Benzoato de sódio	NB20180313	1
Caesar & Loretz GmbH...	Benzoato de sódio	19054114	1
Caesar & Loretz GmbH...	Benzoato de sódio	21001722008	1
Caesar & Loretz GmbH...	Benzoato de sódio	20003762013	1
Caesar & Loretz GmbH...	Benzoato de sódio	21001722003	2
Caesar & Loretz GmbH...	Benzoato de sódio	19054114	1
Caesar & Loretz GmbH...	Benzoato de sódio	21001722003	1
Caesar & Loretz GmbH...	Benzoato de sódio	192296011	1
Caesar & Loretz GmbH/AHD	Benzoato de sódio	20003762013	1
Caesar & Loretz GmbH...	Benzoato de sódio	192296003	1
Caesar & Loretz GmbH/E	Benzoato de sódio	20003762007	1
Caesar & Loretz GmbH...	Benzoato de sódio	19054104	1
Caesar & Loretz GmbH...	Benzoato de sódio	20003762009	1
Caesar & Loretz GmbH/GEHE	Benzoato de sódio	192296003	1
Caesar & Loretz GmbH/Gehe	Benzoato de sódio	192296015	2
Caesar & Loretz GmbH/Gehe	Benzoato de sódio	20003762002	2
Caesar & Loretz GmbH/Gehe	Benzoato de sódio	20003762010	1
Caesar & Loretz GmbH...	Benzoato de sódio	19054114	1
Caesar & Loretz GmbH...	Benzoato de sódio	20003762009	1
Caesar & Loretz GmbH...	Benzoato de sódio	21001722003	1
Caesar & Loretz GmbH...	Benzoato de sódio	21001722008	1
Caesar & Loretz GmbH...	Benzoato de sódio	20003762009	1
Caesar & Loretz GmbH...	Benzoato de sódio	20001291005	1
Caesar & Loretz GmbH...	Benzoato de sódio	20003762013	1
Caesar & Loretz GmbH	Benzoato de sódio	18161201	1
Caesar & Loretz GmbH	Benzoato de sódio	18161211	1
Caesar & Loretz GmbH	Benzoato de sódio	19054104	2
Caesar & Loretz GmbH	Benzoato de sódio	19054114	4
Caesar & Loretz GmbH	Benzoato de sódio	192296003	3
Caesar & Loretz GmbH	Benzoato de sódio	192296011	5
Caesar & Loretz GmbH	Benzoato de sódio	192296015	3
Caesar & Loretz GmbH	Benzoato de sódio	20001291001	3
Caesar & Loretz GmbH	Benzoato de sódio	20001291005	3
Caesar & Loretz GmbH	Benzoato de sódio	20003762003	7
Caesar & Loretz GmbH	Benzoato de sódio	20003762007	6
Caesar & Loretz GmbH	Benzoato de sódio	20003762009	8
Caesar & Loretz GmbH	Benzoato de sódio	20003762013	3
Caesar & Loretz GmbH	Benzoato de sódio	21001722003	5
Caesar & Loretz GmbH	Benzoato de sódio	21001722004	2
Caesar & Loretz GmbH	Benzoato de sódio	21001722006	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Benzoato de sódio	21001722008	7
Caesar & Loretz GmbH	Benzoato de sódio	21001722009	2
Caesar & Loretz GmbH	Benzoato de sódio	21001722020	3
Caesar & Loretz GmbH	Benzoato de sódio	22001421001	3
Caesar & Loretz GmbH	Benzoato de sódio	22001421002	3
Caesar & Loretz Hilden	Benzoato de sódio	18161201	1
Caesar&Lorenz	Benzoato de sódio	20003762015	1
Calo/Krieger	Benzoato de sódio	19054104	1
calo	Benzoato de sódio	17055805	1
Chiesi/Krieger	Benzoato de sódio	17353011	1
EuRho / Noweda	Benzoato de sódio	2009005-01	1
EuRho / Phoenix	Benzoato de sódio	2001018-01	1
EuRho Anzag	Benzoato de sódio	1304024-01	1
EuRho/Sanacorp	Benzoato de sódio	190104302	1
EuRho	Benzoato de sódio	1112006-01	1
EuRho	Benzoato de sódio	2009005-01	1
Euro OCT / Noweda	Benzoato de sódio	1510044-01	1
Euro OTC	Benzoato de sódio	1007019-01	1
Euro OTC	Benzoato de sódio	1112006-01	1
Euro OTC	Benzoato de sódio	1209018-01	4
Euro OTC	Benzoato de sódio	1209018-18	1
Euro OTC	Benzoato de sódio	130402401	2
Euro OTC	Benzoato de sódio	1304024-01	6
Euro OTC	Benzoato de sódio	1307013-01	2
Euro OTC	Benzoato de sódio	1309027-01	2
Euro OTC	Benzoato de sódio	14040-01	1
Euro OTC	Benzoato de sódio	1404011-01	4
Euro OTC	Benzoato de sódio	1409040-01	2
Euro OTC	Benzoato de sódio	15060119-01	1
Euro OTC	Benzoato de sódio	1506019-01	7
Euro OTC	Benzoato de sódio	151004401	4
Euro OTC	Benzoato de sódio	1510044-01	15
Euro OTC	Benzoato de sódio	1510044-0104932321	1
Euro OTC	Benzoato de sódio	15363424	1
Euro OTC	Benzoato de sódio	1602020-01	2
Euro OTC	Benzoato de sódio	1607005-01	5
Euro OTC	Benzoato de sódio	161003701	1
Euro OTC	Benzoato de sódio	1610037-01	3
Euro OTC	Benzoato de sódio	16137112	1
Euro OTC	Benzoato de sódio	1701045	1
Euro OTC	Benzoato de sódio	1701045-01	5
Euro OTC	Benzoato de sódio	170702401	1
Euro OTC	Benzoato de sódio	1707024-01	3
Euro OTC	Benzoato de sódio	171101901	1
Euro OTC	Benzoato de sódio	1711019-01	3
Euro OTC	Benzoato de sódio	1803034-01	3
Euro OTC	Benzoato de sódio	1809005	1
Euro OTC	Benzoato de sódio	180900501	2
Euro OTC	Benzoato de sódio	1809005-01	22
Euro OTC	Benzoato de sódio	1841	1
Euro OTC	Benzoato de sódio	1901043	1
Euro OTC	Benzoato de sódio	190104301	1
Euro OTC	Benzoato de sódio	1901043-01	9
Euro OTC	Benzoato de sódio	1901043-02	11
Euro OTC	Benzoato de sódio	2001018	1
Euro OTC	Benzoato de sódio	200101801	1
Euro OTC	Benzoato de sódio	2001018-01	13
Euro OTC	Benzoato de sódio	20010-18-01	1
Euro OTC	Benzoato de sódio	200900501	1
Euro OTC	Benzoato de sódio	2009005-01	17

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Benzoato de sódio	210901601	1
Euro OTC	Benzoato de sódio	2109016-01	9
Euro OTC	Benzoato de sódio	2109016-02	1
Euro OTC	Benzoato de sódio	2132	1
Euro OTC	Benzoato de sódio	2207025-01	1
Euro OTC	Benzoato de sódio	2302017-01	1
Euro OTC	Benzoato de sódio	2604040V-05	1
Euro Rho	Benzoato de sódio	1803034-01	1
Euro/ Phönix	Benzoato de sódio	1404011-01	1
EuroTOC / Noweda	Benzoato de sódio	130902701	1
Fagron	Benzoato de sódio	12C05-N04	1
Fagron	Benzoato de sódio	12D02-N06	1
Fagron	Benzoato de sódio	12G04-N04	1
Fagron	Benzoato de sódio	12H08-N06	1
Fagron	Benzoato de sódio	12J23-N05	3
Fagron	Benzoato de sódio	13/27b03288805	1
Fagron	Benzoato de sódio	13/27B03288805	1
Fagron	Benzoato de sódio	13/27-B03-288805	1
Fagron	Benzoato de sódio	13/27-B03-288806	2
Fagron	Benzoato de sódio	13C14-N01	4
Fagron	Benzoato de sódio	13C14-NO1	1
Fagron	Benzoato de sódio	13H01-N02	1
Fagron	Benzoato de sódio	13I27-B03288805	1
Fagron	Benzoato de sódio	13I27-B03-288806	3
Fagron	Benzoato de sódio	13l27-B03-288806	1
Fagron	Benzoato de sódio	1412	1
Fagron	Benzoato de sódio	14E12-B07	1
Fagron	Benzoato de sódio	14E12B07296717	1
Fagron	Benzoato de sódio	14E12-B07-306570	1
Fagron	Benzoato de sódio	14E12Bo7296717	1
Fagron	Benzoato de sódio	14E12B07296717	1
Fagron	Benzoato de sódio	1510044-01	2
Fagron	Benzoato de sódio	15363403	1
Fagron	Benzoato de sódio	15B16-B07	1
Fagron	Benzoato de sódio	15B16-B07-306571	2
Fagron	Benzoato de sódio	15B16-B07-308570	1
Fagron	Benzoato de sódio	1602020-01	1
Fagron	Benzoato de sódio	16B23-B06-322528	1
Fagron	Benzoato de sódio	24011401	1
Fagron	Benzoato de sódio	test	1
Fiebig 27.06.13 EK3,34	Benzoato de sódio	1304024-01	1
Gehe	Benzoato de sódio	1404011-01	1
Gehe	Benzoato de sódio	15044102	1
Gehe	Benzoato de sódio	1610037-01	1
Gehe	Benzoato de sódio	1707024-01	2
GEHE	Benzoato de sódio	17137606	1
Gehe	Benzoato de sódio	17317606	1
GEHE	Benzoato de sódio	17353006	2
Gehe	Benzoato de sódio	18161211	7
Gehe	Benzoato de sódio	21001722006	1
Gehe	Benzoato de sódio	2109016-01	1
Gehe	Benzoato de sódio	22001421009	1
Hedinger/Phönix	Benzoato de sódio	15363413	1
Hedinger	Benzoato de sódio	13I27-B03	1
Jenne	Benzoato de sódio	20003762007	1
Kehr	Benzoato de sódio	1701045-01	1
Nachtestung	Benzoato de sódio	300/18	1
Nokun	Benzoato de sódio	17137606	2
Noweda	Benzoato de sódio	1209018-01	1
Noweda	Benzoato de sódio	16137103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Benzoato de sódio	16137112	1
Noweda	Benzoato de sódio	1711019-01	1
Noweda	Benzoato de sódio	18161201	1
Noweda	Benzoato de sódio	189005-01	1
Noweda	Benzoato de sódio	1901043-02	2
Noweda	Benzoato de sódio	192296016	1
Pala	Benzoato de sódio	192296003	1
Phoenix goettin	Benzoato de sódio	13I27-B03-288806	1
Phoenix	Benzoato de sódio	1610037-01	1
Phoenix	Benzoato de sódio	2003762009	1
Phoenix	Benzoato de sódio	2201421009	1
Phönix Gotha	Benzoato de sódio	18161211	2
Phönix Gotha	Benzoato de sódio	19054114	1
Phönix	Benzoato de sódio	1510044/01	1
Phönix	Benzoato de sódio	17137606	1
Phönix	Benzoato de sódio	18161201	1
Phönix	Benzoato de sódio	192296004	2
Phönix	Benzoato de sódio	192296015	1
Phönix	Benzoato de sódio	20001291001	3
sana	Benzoato de sódio	13178635	1
Sanacorp	Benzoato de sódio	192296015	1
Sanacorp	Benzoato de sódio	20001291005	1
Sanacorp	Benzoato de sódio	22001421009	1
Unisan	Benzoato de sódio	1404011-01	1

- 235 131 spectra from 1515 *Apo-Ident* customers from a total of 49 066 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Benzoato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzoato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	790	0	201 294
Type C	0	935	1	235 131

The substance/substance group *Benzoato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2405 %)
Type C	100.0000 % (> 99.9007 %)	99.8932 % (> 99.5726 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20752	22236	20,96	163,63
21607	22363	13,56	160,28
21713	22236	15,14	164,84
21825	21825	0,00	152,10
22236	22236	0,00	166,43
22363	22363	0,00	155,50
22867	22867	0,00	156,41
22997	22997	0,00	156,42
23900	23900	0,00	151,29
25081	25081	0,00	153,98
25379	25379	0,00	213,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Benzocaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20211-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Benzocaína; Benzocainum

Special notes

When selecting the *Benzocaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Benzocaína	9	10	195

Second-stage model

For differentiation of the substance/substance group *Benzocaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Benzocaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	175,06	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Benzocaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Benzocaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzocaína	12341904	20843	40	1411055
Caelo	Benzocaína	13213509	21563	60	1706017
Caelo	Benzocaína	20000972	25195	40	20200513*
Caelo	Benzocaína	22002349	26493	40	20221011*
Caelo	Benzocaína	22002349	26493SI	20	20221011*
Euro OTC	Benzocaína	2207016	26346	40	20221013*
Euro OTC	Benzocaína	2207016	26346SI	20	20221013*
Fagron	Benzocaína	12E04-N06	21083	30	20120607
Fagron	Benzocaína	14G02-B01-306980	23569	40	20140723
Fagron	Benzocaína	16D13-B01-342411	23986	40	1807429
Fagron	Benzocaína	19J11-B11-195266	25172	40	20191031

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 410 spectra of 11 reference samples from the substance/substance group *Benzocaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 552 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 11 reference samples from the substance/substance group *Benzocaína*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzocaína	161740	22641	40
Caelo	Benzocaína	172174	23628	40
Caelo	Benzocaína	182778	24378	40
Caelo	Benzocaína	190220	24531	40
Caelo	Benzocaína	20002741	25616	40
Caelo	Benzocaína	210001141	25642	40
Caelo	Benzocaína	21003052	25854	50
Caelo	Benzocaína	24000752	27221	40
Fagron	Benzocaína	22A15-B10-220491	26183	40
Fagron	Benzocaína	23H08-B12-239118	27190	40
Fagron	Benzocaína	22A15-B10-220491	26183SI	20

- 201 654 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 806 spectra from 418 *Apo-Ident* customers from 209 batches from the substance/substance group *Benzocaína*.

- Among them are spectra of independent samples from 195 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Benzocaína	21003052007	1
	Benzocaína	21J21-B01-216131	1
	Benzocaína	22002349001	10
	Benzocaína	22002349005	3
	Benzocaína	22002349007	1
	Benzocaína	22G25-B01-222567	1
	Benzocaína	22G25-B01-227344	4
	Benzocaína	22H30-B01-231909	1
	Benzocaína	23H08-B12-239118	1
	Benzocaína	B01-2319009	1
	Benzocaína	C0012201014	1
ACM	Benzocaína	KNC1643J15	1
AHD	Benzocaína	16174001	1
Alliance	Benzocaína	22002349001	1
Anzag / Noweda	Benzocaína	1321351	1
Beiersdorf	Benzocaína	15227314	1
Bombastus	Benzocaína	B02-2007200	2
Caelo	Benzocaína		1
Caelo	Benzocaína	1(19022001)	1
Caelo	Benzocaína	10072603	3
Caelo	Benzocaína	11031703	1
Caelo	Benzocaína	11127506	1
Caelo	Benzocaína	11127508	1
Caelo	Benzocaína	1119E-01118	1
Caelo	Benzocaína	12115007	4
Caelo	Benzocaína	12115008	2
Caelo	Benzocaína	12115011	3
Caelo	Benzocaína	12341904	6
Caelo	Benzocaína	12341906	1
Caelo	Benzocaína	13213502	5
Caelo	Benzocaína	13213509	8
Caelo	Benzocaína	13213515	4
Caelo	Benzocaína	13213516	1
Caelo	Benzocaína	13213518	1
Caelo	Benzocaína	13L06-B02	1
Caelo	Benzocaína	13L06-B02-294112	2
Caelo	Benzocaína	14277502	4
Caelo	Benzocaína	1515I-01118	1
Caelo	Benzocaína	15227301	2
Caelo	Benzocaína	15227302	13
Caelo	Benzocaína	15227307	4
Caelo	Benzocaína	15227311	3
Caelo	Benzocaína	15227312	2
Caelo	Benzocaína	15227313	1
Caelo	Benzocaína	15227314	4
Caelo	Benzocaína	15227315	8
Caelo	Benzocaína	15227315I-201016-1	1
Caelo	Benzocaína	15227317	1
Caelo	Benzocaína	15C19-B04-322019	1
Caelo	Benzocaína	15c19-b04-325359	1
Caelo	Benzocaína	16030403	2
Caelo	Benzocaína	16174001	8
Caelo	Benzocaína	16174001I-290517	1
Caelo	Benzocaína	16174005	2
Caelo	Benzocaína	16174007	9
Caelo	Benzocaína	161740075429	1
Caelo	Benzocaína	161740077	1
Caelo	Benzocaína	16174008	1
Caelo	Benzocaína	16174014	16
Caelo	Benzocaína	16174015	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Benzocaína	16174017	6
Caelo	Benzocaína	16174019	12
Caelo	Benzocaína	161740195459	1
Caelo	Benzocaína	16174020	1
Caelo	Benzocaína	16D13-B01_348062	1
Caelo	Benzocaína	16D13-B01-334195	2
Caelo	Benzocaína	16D13-B01-342411	1
Caelo	Benzocaína	16D13-B01-345969	1
Caelo	Benzocaína	16D13-B01-348062	3
Caelo	Benzocaína	18018801	14
Caelo	Benzocaína	18018804	12
Caelo	Benzocaína	18018805	1
Caelo	Benzocaína	18018806	1
Caelo	Benzocaína	18018808	7
Caelo	Benzocaína	18018810	2
Caelo	Benzocaína	18041803	1
Caelo	Benzocaína	18277801	7
Caelo	Benzocaína	18277802	14
Caelo	Benzocaína	18277805	2
Caelo	Benzocaína	18277806	1
Caelo	Benzocaína	18F-B07-190519	1
Caelo	Benzocaína	1902004	1
Caelo	Benzocaína	19022001	10
Caelo	Benzocaína	19022004	11
Caelo	Benzocaína	19022006	3
Caelo	Benzocaína	19031301	1
Caelo	Benzocaína	19210006	1
Caelo	Benzocaína	192710002	2
Caelo	Benzocaína	192710003	23
Caelo	Benzocaína	192710004	3
Caelo	Benzocaína	192710006	21
Caelo	Benzocaína	19271003	1
Caelo	Benzocaína	19271006	1
Caelo	Benzocaína	192829002	1
Caelo	Benzocaína	20000972003	13
Caelo	Benzocaína	20004054001	3
Caelo	Benzocaína	20004055001	17
Caelo	Benzocaína	21000114002	1
Caelo	Benzocaína	21000114004	8
Caelo	Benzocaína	21000114005	9
Caelo	Benzocaína	21000114006	1
Caelo	Benzocaína	21003052004	8
Caelo	Benzocaína	21003052005	1
Caelo	Benzocaína	21003052007	7
Caelo	Benzocaína	2412M-01118	1
Caelo	Benzocaína	3784947	1
Caelo	Benzocaína	5021401	1
Caelo	Benzocaína	6031501	1
Caelo	Benzocaína	718E-01118	1
Caelo	Benzocaína	91062169	1
Caesaer/Jenne	Benzocaína	16174019	1
Caesar & Loretz GmbH...	Benzocaína	18277801	1
Caesar & Loretz GmbH...	Benzocaína	16174019	1
Caesar & Loretz GmbH...	Benzocaína	1927100	1
Caesar & Loretz GmbH...	Benzocaína	20004055001	1
Caesar & Loretz GmbH...	Benzocaína	192710006	3
Caesar & Loretz GmbH...	Benzocaína	192710006	1
Caesar & Loretz GmbH/GEHE	Benzocaína	192710006	1
Caesar & Loretz GmbH...	Benzocaína	18277801	1
Caesar & Loretz GmbH...	Benzocaína	19022001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Ph	Benzocaína	21000114004	2
Caesar & Loretz GmbH…	Benzocaína	21000114005	1
Caesar & Loretz GmbH…	Benzocaína	21003052004	1
Caesar & Loretz GmbH/Sana	Benzocaína	21000114002	2
Caesar & Loretz GmbH…	Benzocaína	192710003	1
Caesar & Loretz GmbH…	Benzocaína	20000972003	2
Caesar & Loretz GmbH…	Benzocaína	505500001	1
Caesar & Loretz GmbH	Benzocaína	18018808	1
Caesar & Loretz GmbH	Benzocaína	18277801	1
Caesar & Loretz GmbH	Benzocaína	18277802	1
Caesar & Loretz GmbH	Benzocaína	18277806	1
Caesar & Loretz GmbH	Benzocaína	19022001	3
Caesar & Loretz GmbH	Benzocaína	19022004	4
Caesar & Loretz GmbH	Benzocaína	19022006	3
Caesar & Loretz GmbH	Benzocaína	192710003	15
CAESAR & LORETZ GMBH	Benzocaína	192710003	2
Caesar & Loretz GmbH	Benzocaína	192710006	4
Caesar & Loretz GmbH	Benzocaína	20000972003	5
Caesar & Loretz GmbH	Benzocaína	20004054001	1
Caesar & Loretz GmbH	Benzocaína	20004055001	12
Caesar & Loretz GmbH	Benzocaína	21000114002	1
Caesar & Loretz GmbH	Benzocaína	21000114004	6
Caesar & Loretz GmbH	Benzocaína	21000114005	2
Caesar & Loretz GmbH	Benzocaína	21003052004	5
Caesar & Loretz GmbH	Benzocaína	21003052007	4
Caesar & Loretz GmbH	Benzocaína	22002349001	1
Caesar & Loretz GmbH	Benzocaína	22002349005	1
Caesar & Loretz Hild…	Benzocaína	192710003	1
Caesar & Loretz Hilden	Benzocaína	18277801	1
Caesar & Loretz/Geil…	Benzocaína	192710003	1
Caesar & Loretz/Geil…	Benzocaína	20004055001	1
Caesar & Loretz/Geil…	Benzocaína	21000114004	1
Caesar Loretz	Benzocaína	192710006	1
Caleo/Phoenix	Benzocaína	20004055001	1
Cealo	Benzocaína	21000114002	1
Changzhou Sunlight P…	Benzocaína	192710003	1
Changzhou/Noweda	Benzocaína	C0011905005	1
Euro OTC	Benzocaína	13L06-B02-297505	1
Euro OTC	Benzocaína	15227313	1
Euro OTC	Benzocaína	15227314	1
Fagrin/Gehe	Benzocaína	15C19-B04	1
Fagron	Benzocaína		1
Fagron	Benzocaína	104210-0001	1
Fagron	Benzocaína	10K02-N01	1
Fagron	Benzocaína	11/22-N03	1
Fagron	Benzocaína	11/22-N3	1
Fagron	Benzocaína	11K08-B40	4
Fagron	Benzocaína	11K08-B40-291840	1
Fagron	Benzocaína	11k08-b40-291841	1
Fagron	Benzocaína	11k08-B40-291841	1
Fagron	Benzocaína	11K08-B40-291841	6
Fagron	Benzocaína	12341904	1
Fagron	Benzocaína	12E014-N06	1
Fagron	Benzocaína	12E04-N06	9
Fagron	Benzocaína	12H10-N06	3
Fagron	Benzocaína	13F06N10	1
Fagron	Benzocaína	13F06-N10	1
Fagron	Benzocaína	13L06-B02	4
Fagron	Benzocaína	13L06-B02_297505	1
Fagron	Benzocaína	13L06-B02-294100	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Benzocaína	13L06-B02-294112	4
Fagron	Benzocaína	13L06-B02-300480	2
Fagron	Benzocaína	13l06-B02-300494	1
Fagron	Benzocaína	13L06-B02-300494	5
Fagron	Benzocaína	13L06Bo2	1
Fagron	Benzocaína	14G02-B01-306980	1
Fagron	Benzocaína	14G02-B01-310324	8
Fagron	Benzocaína	14G02B01318318	1
Fagron	Benzocaína	14G02-B01-318318	3
Fagron	Benzocaína	15227307	1
Fagron	Benzocaína	15C19-B04	1
Fagron	Benzocaína	15C19-B04-308254	1
Fagron	Benzocaína	15C19-B04-316239	3
Fagron	Benzocaína	15C19-B04-322019	7
Fagron	Benzocaína	15c19-b04-325359	1
Fagron	Benzocaína	15C19-B04-325359	3
Fagron	Benzocaína	15C-19-B04-325359	1
Fagron	Benzocaína	16D113-B01-345969	1
Fagron	Benzocaína	16D13	1
Fagron	Benzocaína	16D13_B01_348062	1
Fagron	Benzocaína	16D13-B01	2
Fagron	Benzocaína	16D13B01330168	1
Fagron	Benzocaína	16D13-B01-330168	1
Fagron	Benzocaína	16D13-b01-334195	1
Fagron	Benzocaína	16D13-B01-334195	3
Fagron	Benzocaína	16D13-B01-337264	4
Fagron	Benzocaína	16D13B01341861	2
Fagron	Benzocaína	16D13-B01-341861	2
Fagron	Benzocaína	16d13-b01-342411	1
Fagron	Benzocaína	16D13-B01-342411	5
Fagron	Benzocaína	16D13B01345969	1
Fagron	Benzocaína	16D13-B01-345969	2
Fagron	Benzocaína	16D13-B01-348062	4
Fagron	Benzocaína	18F18-B50	2
Fagron	Benzocaína	18F18B50352167	1
Fagron	Benzocaína	18F18-B50-352167	2
Fagron	Benzocaína	18F18B50352171	1
Fagron	Benzocaína	18F18-B50-352171	6
Fagron	Benzocaína	18F18B50-353577	1
Fagron	Benzocaína	18F18-B50-353577	6
Fagron	Benzocaína	18F18-B50-35377	1
Fagron	Benzocaína	18F18B50355282	1
Fagron	Benzocaína	18F29-B07	1
Fagron	Benzocaína	18F29-B07_190519	1
Fagron	Benzocaína	18f29b07190519	1
Fagron	Benzocaína	18F29B07190519	1
Fagron	Benzocaína	18F29-B07-190519	19
Fagron	Benzocaína	18F-B50	1
Fagron	Benzocaína	18J31-B02	2
Fagron	Benzocaína	18J31-B02-193431	10
Fagron	Benzocaína	18J31-BO2	1
Fagron	Benzocaína	19G02-B04	1
Fagron	Benzocaína	19J11-011-195266	1
Fagron	Benzocaína	19J11-B11	1
Fagron	Benzocaína	19J11-B11-195266	8
Fagron	Benzocaína	19J11-B11-2000500	1
Fagron	Benzocaína	19J11-B11-200500	5
Fagron	Benzocaína	202522/1	1
Fagron	Benzocaína	20817-801-201337	1
Fagron	Benzocaína	20B17B01201337	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Benzocaína	20B17-B01-201337	1
Fagron	Benzocaína	20C09-B02	2
Fagron	Benzocaína	20C09-B02-200720	8
Fagron	Benzocaína	20C09B02-2007200	1
Fagron	Benzocaína	20G27-B05-201740	1
Fagron	Benzocaína	21A26-B18	1
Fagron	Benzocaína	21A26-B18-204192	2
Fagron	Benzocaína	21D13-B03-210845	3
Fagron	Benzocaína	21G17-B07-214449	1
Fagron	Benzocaína	21J21-B01	1
Fagron	Benzocaína	21J21-B01-216131	1
Fagron	Benzocaína	21J21-B01-218075	3
Fagron	Benzocaína	21J21-BO1-216131	1
Fagron	Benzocaína	22G25-B01-222567	1
Fagron	Benzocaína	2OG27-BO5-201740	1
Fagron	Benzocaína	400313	1
Fagron	Benzocaína	4413E-01118	1
Fagron	Benzocaína	581015	2
Fagron	Benzocaína	B01-2005307	1
Fagron	Benzocaína	B02-2007200	2
Fagron	Benzocaína	B071905109	1
Fagron	Benzocaína	B11-1952606	1
Fagron	Benzocaína	B11-2005000	1
Fagron	Benzocaína	BZ-08/11-12	1
Fagron	Benzocaína	BZ-27/1112	1
Fagron	Benzocaína	C0011803001	1
Fagron	Benzocaína	C0011911003	1
Fagron	Benzocaína	C0012106001	3
Fargon/Sana	Benzocaína	11K08-290049	1
Fargon/Sanacorp	Benzocaína	20C09-B02_200720	1
Fargon	Benzocaína	12H10-N06	1
Fargron	Benzocaína	13L06-B02-294112	1
Fiebig	Benzocaína	13L06-B02-300494	1
Fiebig	Benzocaína	15C19-B04-325359	1
Fiebig	Benzocaína	18018801	1
Fragon	Benzocaína	B02-2007200	1
Gehe	Benzocaína	111214	1
Gehe	Benzocaína	15C19-B04	1
Gehe	Benzocaína	16D13-B01-337264	1
Gehe	Benzocaína	18018801	1
Gehe	Benzocaína	18018808	1
Gehe	Benzocaína	18277801	1
Gehe	Benzocaína	18J31-B02-193431	1
Gehe	Benzocaína	20004055001	1
Gehe	Benzocaína	22002349005	1
Gehe	Benzocaína	22G25-B01-227344	1
Geibo	Benzocaína	22G25-B01-227344	1
Jenne / Fargon	Benzocaína	16D13-B01-337264	1
Jenne	Benzocaína	21003052004	1
Kehr	Benzocaína	15C19-B04-325359	1
Kehr	Benzocaína	16D13-B01-330168	1
L12	Benzocaína	16D13-B01-348062	1
Mömerzheim	Benzocaína	18018804	2
Noweda	Benzocaína	15227313	1
Noweda	Benzocaína	18018804	1
Noweda	Benzocaína	192710003	2
Noweda	Benzocaína	20000972003	1
Noweda	Benzocaína	21000114005	1
Noweda	Benzocaína	22002349007	1
otto geilenkirchen	Benzocaína	192710006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Benzocaína	12H10-N06	1
Phoenix	Benzocaína	19022001	2
Phoenix	Benzocaína	19022006	1
Phoenix	Benzocaína	192710006	1
Phönix	Benzocaína	13F06-N10	1
Phönix	Benzocaína	20004055001	1
s.Prüfprotokoll	Benzocaína		1
Sanacorp W.E:07.01.1...	Benzocaína	13213502	1
Sanacorp	Benzocaína	13213502	1
Sanacorp	Benzocaína	13213506	1
Sanacorp	Benzocaína	18018801	1

- 235 261 spectra from 1515 *Apo-Ident* customers from a total of 49 053 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Benzocaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzocaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	430	0	201 654
Type C	0	803	3	235 261

The substance/substance group *Benzocaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	99.6278 % (> 99.2556 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20843	20843	0,00	286,62
21083	21563	56,62	270,56
21563	21563	0,00	283,55
23569	23986	6,59	286,02
23986	23986	0,00	285,82
25172	21563	11,32	283,80
25195	25195	0,00	285,01
26346	26346	0,00	280,75
26493	26493	0,00	280,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Besilato de anlodipino**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005976-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Besilato de anlodipino; Amlodipini besilas; Anlodipino, besilato

Special notes

When selecting the *Besilato de anlodipino* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Besilato de anlodipino	4	1	1

Second-stage model

For differentiation of the substance/substance group *Besilato de anlodipino* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Besilato de anlodipino* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	123,28	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Besilato de anlodipino* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Besilato de anlodipino*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Besilato de anlodipino	21J12-B20-217787	26064	40	2301087
Fagron	Besilato de anlodipino	23F02-B01-233301	26980	40	20230705
Fagron	Besilato de anlodipino	23K14-B07-233516	27176	40	20231205
Hetero Dru…	Besilato de anlodipino	AL22090086	26403	40	20220929
Hetero Dru…	Besilato de anlodipino	AL22090086	26403SI	20	20220929

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Besilato de anlodipino*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 782 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 3 reference samples from the substance/substance group *Besilato de anlodipino*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Besilato de anlodipino	21L15-B03-220098	26073	40
Fagron	Besilato de anlodipino	21J12-B20-217787	26064SI†	10
Fagron	Besilato de anlodipino	21L15-B03-220098	26073SI	10

- 202 024 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Besilato de anlodipino*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Besilato de anlodipino	21L15-B03-220098	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Besilato de anlodipino* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Besilato de anlodipino* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	60	0	202 024
Type C	0	1	0	236 066

The substance/substance group *Besilato de anlodipino* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26064	26064	0,00	281,22
26403	26064	8,81	279,59
26980	26064	7,33	276,54
27176	26064	5,50	276,69

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Betaína monoidratada**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20498-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betaína monoidratada; Betainum monohydricum

Special notes

When selecting the *Betaína monoidratada* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Betaína monoidratada	4	1	4

Second-stage model

For differentiation of the substance/substance group *Betaína monoidratada* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Betaína monoidratada* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	132,83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Betaína monoidratada* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Betaína monoidratada*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Betaína monoidratada	12336602	20991	40	1403327
Fagron	Betaína monoidratada	14I26-B06-309878	21956	60	20141212
Fagron	Betaína monoidratada	18H13-B01-355585	24585	40	20180907
Fagron	Betaína monoidratada	20J26-B02-201459	25480	40	20201104

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Betaína monoidratada*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 782 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Betaína monoidratada*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betaína monoidratada	16H03-B04-330370	23092	40
Fagron	Betaína monoidratada	16H03-B04-330370	23378	40

- 202 004 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Betaína monoidratada*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Betaína monoidratada	14A14-B02-292983	1
Caelo	Betaína monoidratada	4312172831	1
Fagron	Betaína monoidratada	16H03-B04	1
Fagron	Betaína monoidratada	16H03-B04-330370	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Betaína monoidratada* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betaína monoidratada* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	80	0	202 004
Type C	0	4	0	236 063

The substance/substance group *Betaína monoidratada* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20991	20991	0,00	271,72
21956	20991	6,48	271,34
24585	20991	11,29	266,66
25480	20991	13,89	271,81

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Betametasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20943-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betametasona; Betamethasonum

Special notes

When selecting the *Betametasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Betametasona	5	3	38

Second-stage model

For differentiation of the substance/substance group *Betametasona* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Betametasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	91,24	–
⋮	⋮	⋮
Metilprednisolona	>50	52,42
Dexametasona	>50	57,14
Fluocinolona acetonida	>50	58,62
Triancinolona acetonido	>50	64,54
Prednisolona	>50	67,35
Tirotricina	>50	90,23
Gramicidina	>50	153,50

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Betametasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Betametasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Betametasona	12D26-N08	20943	40	1402096
Fagron	Betametasona	13H08-N06	21579	60	1411037
Fagron	Betametasona	11H31-B06-288219	22493	40	1608324
Fagron	Betametasona	20A27-F07-368847	25173	40	20200320
Fagron	Betametasona	23F15-B13-227908	26981	40	20230817

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Betametasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 742 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Betametasona*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betametasona	14C13-B02-296165	22897	40
Fagron	Betametasona	15L09-B05-324091	22904	40
Fagron	Betametasona	21K15-B08-213853	26062	40
Fagron	Betametasona	21K15-B08-213853	26062SI	40

- 201 924 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 53 spectra from 38 *Apo-Ident* customers from 40 batches from the substance/substance group *Betametasona*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
BASF/Phönix	Betametasona	ZBtBY13004	1
Caelo	Betametasona	11/14-N02	1
Caelo	Betametasona	16107-B01-341871	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betametasona	11/14-N02	1
Fagron	Betametasona	11H31-B06-288217	1
Fagron	Betametasona	12B20-N05	2
Fagron	Betametasona	12D26-N08	1
Fagron	Betametasona	12D26-N08	1
Fagron	Betametasona	12J01-N02	1
Fagron	Betametasona	14C13-B02	2
Fagron	Betametasona	14C13-B02-296154	1
Fagron	Betametasona	14C13-B02-296164	2
Fagron	Betametasona	14C13-B02-305561	1
Fagron	Betametasona	14c13-bo2-305561	1
Fagron	Betametasona	15L09-B05	1
Fagron	Betametasona	15L09-B05_322119	1
Fagron	Betametasona	16I07-B01-341871	3
Fagron	Betametasona	1810B02-353535	1
Fagron	Betametasona	18I10-B02-353535	1
Fagron	Betametasona	18I10-B02-353536	2
Fagron	Betametasona	18I10-B02-355063	2
Fagron	Betametasona	18I10-B02-357418	1
Fagron	Betametasona	18l10-B02-355063	1
Fagron	Betametasona	20A27-F07	1
Fagron	Betametasona	20A27-F07-368846	2
Fagron	Betametasona	20A27-F07-368847	1
Fagron	Betametasona	20A27-F07-370552	1
Fagron	Betametasona	21K15-B08-213852	1
Fagron	Betametasona	9071304	1
Fagron	Betametasona	9J26-N08	1
Fagron	Betametasona	9K25-N13	1
Fagron	Betametasona	BT-191101	1
Fagron	Betametasona	F07-3705501	1
Fagron	Betametasona	ZBTBY15002	1
Fargon	Betametasona	20A27-F07-370551	1
Fiebig	Betametasona	12J01-120301-m1	1
Gehe amax	Betametasona	18/10-B02-353535	1
Gehe	Betametasona	15L09-B05-319353	1
Huan Yuxin Pharmaceutics	Betametasona	20A27-F07-370551	1
Hunan Yuxin Pharmace…	Betametasona	20A27-F07-372113	1
Noweda	Betametasona	12B20-N05	1
Noweda	Betametasona	M-XO1-120301m1	1
Phönix	Betametasona	12B20-N05	1
Symbiotec Pharmalab …	Betametasona	14C13-B02	1
Unisan	Betametasona	Retest09K25-N13	1

- 236 014 spectra from 1515 *Apo-Ident* customers from a total of 49 218 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Betametasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betametasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	160	0	201 924
Type C	0	48	5	236 014

The substance/substance group *Betametasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	90.5660 % (> 84.9057 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20943	20943	0,00	116,34
21579	21579	0,00	128,89
22493	22493	0,00	127,56
25173	21579	26,39	133,76
26981	21579	22,01	135,26

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bicarbonato de amônio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20166-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bicarbonato de amônio; Ammonii hydrogencarbonas

Special notes

When selecting the *Bicarbonato de amônio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bicarbonato de amônio	2	1	13

Second-stage model

For differentiation of the substance/substance group *Bicarbonato de amônio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bicarbonato de amônio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloreto de alumínio hexa-hidratado	143,02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bicarbonato de amônio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bicarbonato de amônio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bicarbonato de amônio	182108	24268	40	20180926*
Caelo	Bicarbonato de amônio	23002439	27078	31	20230929*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 71 spectra of 2 reference samples from the substance/substance group *Bicarbonato de amônio*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 891 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 70 spectra of 2 reference samples from the substance/substance group *Bicarbonato de amônio*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bicarbonato de amônio	21001324	25811	50
Caelo	Bicarbonato de amônio	23002439	27078SI†	20

- 202 014 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 11 *Apo-Ident* customers from 13 batches from the substance/substance group *Bicarbonato de amônio*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Bicarbonato de amônio	11145612	2
Caelo	Bicarbonato de amônio	12022308	2
Caelo	Bicarbonato de amônio	12322201	1
Caelo	Bicarbonato de amônio	12322204	1
Caelo	Bicarbonato de amônio	13104601	1
Caelo	Bicarbonato de amônio	13104611	1
Caelo	Bicarbonato de amônio	23011404	1
Caelo	Bicarbonato de amônio	24101202	1
Caelo	Bicarbonato de amônio	25111308	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bicarbonato de amônio	3091204	1
Caelo	Bicarbonato de amônio	3712Q-01103	1
Caelo	Bicarbonato de amônio	72715338	1
Caelo	Bicarbonato de amônio	9139402	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bicarbonato de amônio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bicarbonato de amônio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	71	0	152 891
Type B	0	50	20	202 014
Type C	0	15	0	236 052

The substance/substance group *Bicarbonato de amônio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 91.5493 %)
Type B	100.0000 % (> 99.9912 %)	71.4286 % (> 67.1429 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24268	24268	0,00	202,22
27078	27078	0,00	211,61

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bifonazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20810-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bifonazol; Bifonazolum

Special notes

When selecting the *Bifonazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bifonazol	8	5	75

Second-stage model

For differentiation of the substance/substance group *Bifonazol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bifonazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clotrimazol	30,04	–
Metoxisaleno	145,52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bifonazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bifonazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bifonazol	15152701	22906	40	20150703
Caelo	Bifonazol	15152702	22907	40	20150703
Caelo	Bifonazol	15152702	22955	40	20150703
Caelo	Bifonazol	151527	23364	40	20150703*
Euro OTC	Bifonazol	1206027-01	20810	40	1312397
Euro OTC	Bifonazol	1401031-01	21631	60	20140220
Euro OTC	Bifonazol	1510001	22253	60	20151203*
Fagron	Bifonazol	12G11-N09	20820	40	20120807
Fagron	Bifonazol	16D07-B10-324381	22941	40	20160419

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Bifonazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Bifonazol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bifonazol	182771	24365	40
Caelo	Bifonazol	22001498	26738	40
Euro OTC	Bifonazol	1703041	23395	40
Euro OTC	Bifonazol	1806008	24161	40
Fagron	Bifonazol	22C23-B03-219763	26376	40
Caelo	Bifonazol	22001498	26738SI	20
Fagron	Bifonazol	22C23-B03-219763	26376SI	20

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 211 spectra from 81 *Apo-Ident* customers from 84 batches from the substance/substance group *Bifonazol*.

- Among them are spectra of independent samples from 75 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bifonazol	21B18-B03-228686	2
	Bifonazol	22001498010	1
	Bifonazol	22C23-B03-223797	2
	Bifonazol	22L06-B10-223798	2
Caelo	Bifonazol	13I09-N07	1
Caelo	Bifonazol	14k10-B01-312067	1
Caelo	Bifonazol	15152701	6
Caelo	Bifonazol	16J03-B08-331029	1
Caelo	Bifonazol	1703041-01	2
Caelo	Bifonazol	18009702	9
Caelo	Bifonazol	18009704	4
Caelo	Bifonazol	18009705	1
Caelo	Bifonazol	18277103	1
Caelo	Bifonazol	18277104	1
Caelo	Bifonazol	19287504	1
Caelo	Bifonazol	19287505	2
Caelo	Bifonazol	20003802002	3
Caesar & Loretz GmbH...	Bifonazol	18277104	1
Caesar & Loretz GmbH...	Bifonazol	19287505	1
Caesar & Loretz GmbH	Bifonazol	18277104	1
Caesar & Loretz GmbH	Bifonazol	19287505	2
Caesar & Loretz GmbH	Bifonazol	20003802002	2
Erregierre S.p.A	Bifonazol	A200003	2
Euro OTC	Bifonazol	1206027-01	2
Euro OTC	Bifonazol	1206027-02	1
Euro OTC	Bifonazol	13G10N02	1
Euro OTC	Bifonazol	1510001-02	6
Euro OTC	Bifonazol	16703-B08-333937	1
Euro OTC	Bifonazol	170304101	1
Euro OTC	Bifonazol	1703041-01	5
Euro OTC	Bifonazol	18041814	1
Euro OTC	Bifonazol	1806008-01	12
Euro OTC	Bifonazol	18065008-01	1
Euro Rho/Jenne	Bifonazol	1806008-011	1
Fagron	Bifonazol		2
Fagron	Bifonazol	11F20-N06	1
Fagron	Bifonazol	12D17-N02	3
Fagron	Bifonazol	12E29-N03	5
Fagron	Bifonazol	12G11-N09	2
Fagron	Bifonazol	13G10-N02	2
Fagron	Bifonazol	14C28-B03-292388	1
Fagron	Bifonazol	14C28-B03-292389	1
Fagron	Bifonazol	14K10-B01-300541	6
Fagron	Bifonazol	14K10-B01-306783	5
Fagron	Bifonazol	14K10-B01-308349	2
Fagron	Bifonazol	14K10-B01-312067	2
Fagron	Bifonazol	14K10-B01-316618	1
Fagron	Bifonazol	15/18-B04-320085	1
Fagron	Bifonazol	1518-B04-316619	1
Fagron	Bifonazol	15I18-B04-316619	1
Fagron	Bifonazol	1607-B10-324380	1
Fagron	Bifonazol	16D07-B10-321576	2
Fagron	Bifonazol	16D07-B10-324380	3
Fagron	Bifonazol	16D07-B10-324381	6
Fagron	Bifonazol	16D07-B10-32480	1
Fagron	Bifonazol	16j03-b08-327046	2
Fagron	Bifonazol	16J03-B08-327046	4
Fagron	Bifonazol	16J03-B08-331029	2
Fagron	Bifonazol	16J03-B08-333936	2
Fagron	Bifonazol	16J03-B08-333937	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bifonazol	18A15-B05	1
Fagron	Bifonazol	18A15-B05_344514	1
Fagron	Bifonazol	18A15-B05-344515	4
Fagron	Bifonazol	18A15-B05-347176	2
Fagron	Bifonazol	18A15-B05-350644	1
Fagron	Bifonazol	18A15-B05-353060	2
Fagron	Bifonazol	18A15-B05-357230	1
Fagron	Bifonazol	18A15-B05-357781	2
Fagron	Bifonazol	18A15-B05-358736	2
Fagron	Bifonazol	18A15-B05-362358	1
Fagron	Bifonazol	18A15-B5-34716	1
Fagron	Bifonazol	19E06B01363093	1
Fagron	Bifonazol	19E06-B01-363093	7
Fagron	Bifonazol	19E06-B01-367109	2
Fagron	Bifonazol	19L04-F02-369242	8
Fagron	Bifonazol	19L-F02-369242	1
Fagron	Bifonazol	20L03-F03-375885	7
Fagron	Bifonazol	20L03-F03-375887	1
Fagron	Bifonazol	21B18-B03-215543	4
Fagron	Bifonazol	22C23-B03-223797	1
Fagron	Bifonazol	A160002	1
Fagron	Bifonazol	A170003	1
Fagron	Bifonazol	A190005	1
Fagron	Bifonazol	A200003	1
Fagron	Bifonazol	B05-3623508	1
Fagron	Bifonazol	f02-3671100	2
Fargon	Bifonazol	14k10-b01-300541	1
Gehe	Bifonazol	13D12-N11	1
Gehe	Bifonazol	15152703	1
Gehe	Bifonazol	19L04-F02-369242	1
Gehe	Bifonazol	20003802009	1
Noweda	Bifonazol	18A15-B05-344514	1
Sanacorp	Bifonazol	19287505	1
Sanacorp	Bifonazol	19E06-B01	1

- 235 856 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bifonazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bifonazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	240	0	201 844
Type C	0	208	3	235 856

The substance/substance group *Bifonazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.5782 % (> 97.1564 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20810	20810	0,00	64,26
20820	23364	12,22	60,98
21631	20810	9,03	66,72
22253	22253	0,00	66,68
22906	22253	6,50	61,71
22907	23364	4,80	63,36
22941	23364	4,40	62,83
22955	23364	3,06	63,13
23364	23364	0,00	64,04

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Biotina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20414-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Biotina; Biotinum

Special notes

When selecting the *Biotina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Biotina	8	16	56

Second-stage model

For differentiation of the substance/substance group *Biotina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Biotina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	124,18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Biotina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Biotina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Biotina	16164313	22901	40	20160616
Caelo	Biotina	16164313	22902	40	20160216
Caelo	Biotina	163432	23029	40	20170119*
Caelo	Biotina	163432	23063	40	20170119*
Euro OTC	Biotina	1402028-01	21632	60	20140404
Euro OTC	Biotina	1508030	21904	60	20150925*
Euro OTC	Biotina	1610003	22855	40	20161110*
Euro OTC	Biotina	2009044	25536	40	20210215*
Fagron	Biotina	13K29-N02	21221	40	20131204
Fagron	Biotina	17K20-B03-351524	24694	40	20180108

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Biotina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

batches.

- 152 522 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 710 spectra of 19 reference samples from the substance/substance group *Biotina*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Biotina	173152	23829	40
Caelo	Biotina	183009	24372	40
Caelo	Biotina	21003208	25850	50
Caelo	Biotina	24000895	27224	40
Caelo	Biotina	23003236	27228	40
Euro OTC	Biotina	1603017	22507	40
Euro OTC	Biotina	1708007	23728	40
Euro OTC	Biotina	1802022	23955	40
Euro OTC	Biotina	1903020	24612	40
Euro OTC	Biotina	1903019	24631	40
Euro OTC	Biotina	2005032	25420	40
Euro OTC	Biotina	2110003	25875	50
Euro OTC	Biotina	2306005	26934	40
Euro OTC	Biotina	2311005	27146	40
Fagron	Biotina	22C02-B01-217682	26157	40
Fagron	Biotina	24D08-B01-236877	27374	40
Euro OTC	Biotina	2110003	25875SI	10
Euro OTC	Biotina	2306005	26934SI	20
Fagron	Biotina	22C02-B01-217682	26157SI	20

- 201 374 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 123 spectra from 38 *Apo-Ident* customers from 60 batches from the substance/substance group *Biotina*.

- Among them are spectra of independent samples from 56 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Biotina	2009044-03	1
	Biotina	21002482008	1
	Biotina	22C02-B01-224530	1
	Biotina	22CD2-BD1-217682	1
	Biotina	2306005-02	3
	Biotina	24000895001	1
Caelo	Biotina	12A23-N03	1
Caelo	Biotina	13K29-N02	2
Caelo	Biotina	1402028-01	2
Caelo	Biotina	1610003-02	1
Caelo	Biotina	1708007-01	2
Caelo	Biotina	17D28-B07-334630	1
EuRho	Biotina	1802022-01	1
Euro OTC	Biotina	10061709	1
Euro OTC	Biotina	1111039-02	1
Euro OTC	Biotina	1301026-01	3
Euro OTC	Biotina	1402028-01	2
Euro OTC	Biotina	1411047-01	3
Euro OTC	Biotina	1508030-01	2
Euro OTC	Biotina	1603017-01	1
Euro OTC	Biotina	161000301	1
Euro OTC	Biotina	1610003-01	6
Euro OTC	Biotina	170800701	1
Euro OTC	Biotina	1708007-01	8
Euro OTC	Biotina	180202201	6
Euro OTC	Biotina	1802022-01	4
Euro OTC	Biotina	1802022-02	3
Euro OTC	Biotina	1802022-03	1
Euro OTC	Biotina	1903019-01	5
Euro OTC	Biotina	190302001	1
Euro OTC	Biotina	1903020-01	4
Euro OTC	Biotina	2009044-01	14
Euro OTC	Biotina	2009044-02	1
Euro OTC	Biotina	2041517	1
Euro OTC	Biotina	2110003	1
Euro OTC	Biotina	2110003-01	7
Euro OTC	Biotina	24011801	1
Euro OTC	Biotina	2417Q-01100	1
Euro OTC	Biotina	28071506	1
Euro OTC	Biotina	2818Q-01100	1
Euro OTC	Biotina	3021501	1
Euro OTC	Biotina	5121812	1
Fagron	Biotina	12111302	1
Fagron	Biotina	12A23-N03	1
Fagron	Biotina	12C14-N01	1
Fagron	Biotina	13081203	1
Fagron	Biotina	13111202	1
Fagron	Biotina	14d04-b07-292963	1
Fagron	Biotina	17k20-B03-351524	1
Fagron	Biotina	17K20-B03-351524	1
Fagron	Biotina	19E22-B01-363404	1
Fagron	Biotina	20110634	1
Fagron	Biotina	20K09-F02-375271	1
Fagron	Biotina	20K09-F02-375272	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Biotina	22C02-B01-217682	1
Fagron	Biotina	F03-3775400	1
Fagron	Biotina	UE01704007	1
Fagron	Biotina	UE01807006	1
Fagron	Biotina	UE02005010	1
Fagron	Biotina	UE02005015	1
Gatt-Koller	Biotina	1634211	1
kögl	Biotina	17315206	1
KÖGL	Biotina	17315212	1
privat	Biotina	20171208-05-100	1

- 235 944 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Biotina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Biotina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	710	0	201 374
Type C	0	123	0	235 944

The substance/substance group *Biotina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1549 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.1220 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21221	21904	13,84	158,01
21632	21904	6,46	161,10
21904	21904	0,00	163,16
22855	22855	0,00	164,46
22901	21904	4,37	164,60
22902	21904	4,93	165,10
23029	23029	0,00	166,30
23063	23063	0,00	165,56
24694	23029	11,48	166,91
25536	25536	0,00	165,10

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bitartarato de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20509-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bitartarato de potássio; Kalii hydrogentartras

Special notes

When selecting the *Bitartarato de potássio* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bitartarato de potássio	5	3	40

Second-stage model

For differentiation of the substance/substance group *Bitartarato de potássio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bitartarato de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloreto de alumínio hexa-hidratado	86,85	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bitartarato de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bitartarato de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bitartarato de potássio	11345805	20772	40	20120103
Caelo	Bitartarato de potássio	15354609	23193	40	20151030
Caelo	Bitartarato de potássio	170656	23285	40	20170511*
Caelo	Bitartarato de potássio	182051	24763	40	20180903*
Caelo	Bitartarato de potássio	22001645	26247	40	20220701*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Bitartarato de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Bitartarato de potássio*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bitartarato de potássio	17065604	23414	40
Caelo	Bitartarato de potássio	17065603	23709	40
Caelo	Bitartarato de potássio	20001056	25288	40
Caelo	Bitartarato de potássio	22001645	26247SI†	20

- 201 944 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 72 spectra from 41 *Apo-Ident* customers from 41 batches from the substance/substance group *Bitartarato de potássio*.
- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bären Apotheke	Bitartarato de potássio	15354613	1
Caelo	Bitartarato de potássio	11127417	1
Caelo	Bitartarato de potássio	11345807	1
Caelo	Bitartarato de potássio	13030006	2
Caelo	Bitartarato de potássio	13133104	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bitartarato de potássio	13133114	1
Caelo	Bitartarato de potássio	13133120	2
Caelo	Bitartarato de potássio	13133126	1
Caelo	Bitartarato de potássio	14115208	1
Caelo	Bitartarato de potássio	15081005	1
Caelo	Bitartarato de potássio	15081008	2
Caelo	Bitartarato de potássio	15081010	3
Caelo	Bitartarato de potássio	1534609	1
Caelo	Bitartarato de potássio	15354601	1
Caelo	Bitartarato de potássio	15354604	3
Caelo	Bitartarato de potássio	15354609	3
Caelo	Bitartarato de potássio	15354613	2
Caelo	Bitartarato de potássio	15354614	2
Caelo	Bitartarato de potássio	160514b	1
Caelo	Bitartarato de potássio	17061303	1
Caelo	Bitartarato de potássio	17065603	2
Caelo	Bitartarato de potássio	18205103	2
Caelo	Bitartarato de potássio	18205104	1
Caelo	Bitartarato de potássio	18205106	1
Caelo	Bitartarato de potássio	18205107	1
Caelo	Bitartarato de potássio	20004282003	1
Caelo	Bitartarato de potássio	23062015A	1
Caelo	Bitartarato de potássio	90573259	1
Caesar & Loretz GmbH	Bitartarato de potássio	17366002	1
Caesar & Loretz GmbH	Bitartarato de potássio	182051002	1
Caesar & Loretz GmbH	Bitartarato de potássio	18205101	7
Caesar & Loretz GmbH	Bitartarato de potássio	18205105	1
Caesar & Loretz GmbH	Bitartarato de potássio	18205107	1
Caesar & Loretz GmbH	Bitartarato de potássio	20001056003	1
Caesar & Loretz GmbH	Bitartarato de potássio	20001056005	1
Caleo/ Noweda	Bitartarato de potássio	18205103	1
Gehe	Bitartarato de potássio	11345808	1
Hänseler	Bitartarato de potássio		6
Lamotte/Phönix	Bitartarato de potássio	17065602	1
phönix	Bitartarato de potássio	15354604	1
Phönix	Bitartarato de potássio	20004282003	1
Sanacorp	Bitartarato de potássio	14115208	3
Sanacorp	Bitartarato de potássio	15354609	1
Sanacorp	Bitartarato de potássio	20001056003	1
Sanacorp	Bitartarato de potássio	20001056005	1

- 235 995 spectra from 1515 *Apo-Ident* customers from a total of 49 217 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bitartarato de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bitartarato de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	140	0	201 944
Type C	0	71	1	235 995

The substance/substance group *Bitartarato de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	98.6111 % (> 94.4444 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20772	23285	9,17	176,58
23193	23285	5,79	178,69
23285	23285	0,00	174,28
24763	24763	0,00	175,22
26247	26247	0,00	176,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Brometo de butilescopolamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20766-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Brometo de butilescopolamina; Butilbrometo de escopolamina; Butilescopolamina, brometo; Escopolamina, butilbrometo; Hyoscini butylbromidum

Special notes

When selecting the *Brometo de butilescopolamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Brometo de butilescopolamina	6	4	2

Second-stage model

For differentiation of the substance/substance group *Brometo de butilescopolamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Brometo de butilescopolamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	115,97	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Brometo de butilescopolamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Brometo de butilescopolamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Brometo de butilescopolamina	12K01-N07	20766	40	1406057
Fagron	Brometo de butilescopolamina	12K01-N07	20897	40	20121102
Fagron	Brometo de butilescopolamina	13K22-N03	21049	40	20131126
Fagron	Brometo de butilescopolamina	15I09-B04-312245	21954	60	20150921
Fagron	Brometo de butilescopolamina	18A03-B01-352889	24576	40	20180122
Fagron	Brometo de butilescopolamina	21K26-B03-221816	26294	40	20220226
Fagron	Brometo de butilescopolamina	23G12-B15-233752	26982	40	20230808

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Brometo de butilescopolamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 662 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Brometo de butilescopolamina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Brometo de butilescopolamina	15I09-B04-316806	22344	60
Fagron	Brometo de butilescopolamina	16I20-B08-326942	22903	40
Fagron	Brometo de butilescopolamina	20C24-F01-369374	25482	40
Fagron	Brometo de butilescopolamina	21B12-F02-377294	25911	40
Fagron	Brometo de butilescopolamina	16I20-B08-326942	22937	40
Fagron	Brometo de butilescopolamina	21B12-F02-377294	25911SI	10
Fagron	Brometo de butilescopolamina	21K26-B03-221816	26294SI†	20
Fagron	Brometo de butilescopolamina	23G12-B15-233752	26982SI†	20

- 201 814 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Brometo de butilescopolamina*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Fagron	Brometo de butilescopolamina	16I20-B08-326942	12
Fagron	Brometo de butilescopolamina	18A03-B01-352889	2
Fagron	Brometo de butilescopolamina	21B12-F02-377294	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Brometo de butilescopolamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Brometo de butilescopolamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	270	0	201 814
Type C	0	15	0	236 052

The substance/substance group *Brometo de butilescopolamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20766	20766	0,00	249,58
20897	20766	43,50	247,83
21049	20766	9,22	247,88
21954	20766	8,99	248,71

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24576	20766	20,20	248,95
26294	20766	18,94	249,50
26982	20766	15,19	250,25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Brometo de glicopirrônio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	23076-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Brometo de glicopirrônio; Glicopirrônio, brometo; Glycopyrronii bromidum

Special notes

When selecting the *Brometo de glicopirrônio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Brometo de glicopirrônio	6	3	3

Second-stage model

For differentiation of the substance/substance group *Brometo de glicopirrônio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Brometo de glicopirrônio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Propionato de clobetasol	111,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Brometo de glicopirrônio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Brometo de glicopirrônio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Brometo de glicopirrônio	16E09-B08-331027	23076	40	1707615
Fagron	Brometo de glicopirrônio	16E09-B08-331027	23077	40	20160530
Fagron	Brometo de glicopirrônio	18C30-B07-350744	24183	40	20180502
Fagron	Brometo de glicopirrônio	18G25-B01-356318	24575	40	20180907
Fagron	Brometo de glicopirrônio	20B03-F12-368270	25440	40	20200228
Fagron	Brometo de glicopirrônio	22B10-B05-219477	26285	40	20220624
Fagron	Brometo de glicopirrônio	23C02-B07-228663	26669	40	20230321

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Brometo de glicopirrônio*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Brometo de glicopirrônio*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Brometo de glicopirrônio	17D28-B04-341606	23939	40
Fagron	Brometo de glicopirrônio	21A08-F03-376481	25742	50
Fagron	Brometo de glicopirrônio	21H13-B22-215731	25906	40
Fagron	Brometo de glicopirrônio	21H13-B22-215731	25906SI	10
Fagron	Brometo de glicopirrônio	22B10-B05-219477	26285SI†	20
Fagron	Brometo de glicopirrônio	23C02-B07-228663	26669SI†	20

- 201 904 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Brometo de glicopirrônio*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Brometo de glicopirrônio	18C30-B07-350744	3
Fagron	Brometo de glicopirrônio	21A08-F03-376481	2
Fagron	Brometo de glicopirrônio	21H13-B22-215731	1
Fagron	Brometo de glicopirrônio	21H13-B22-217575	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 060 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Brometo de glicopirrônio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Brometo de glicopirrônio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	180	0	201 904
Type C	0	7	0	236 060

The substance/substance group *Brometo de glicopirrônio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23076	23076	0,00	131,48
23077	23076	2,68	131,10
24183	23076	6,39	130,08
24575	23076	10,09	129,80
25440	23076	12,48	129,34
26285	23076	13,49	128,19
26669	23076	14,31	128,57

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Brometo de ipratrópio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20911-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Brometo de ipratrópio; Ipratropii bromidum; Ipratrópio, brometo

Special notes

When selecting the *Brometo de ipratrópio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Brometo de ipratrópio	5	3	12

Second-stage model

For differentiation of the substance/substance group *Brometo de ipratrópio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Brometo de ipratrópio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	133,18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Brometo de ipratrópio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Brometo de ipratrópio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Brometo de ipratrópio	12C15-N01	20911	40	1403675
Fagron	Brometo de ipratrópio	12K01-N08	21272	40	20121025
Fagron	Brometo de ipratrópio	18H30-B09-359179	24947	40	20180918
Fagron	Brometo de ipratrópio	21E27-B06-213614	25903	40	20210908
Fagron	Brometo de ipratrópio	23C07-B08-230203	26897	40	20230418

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Brometo de ipratrópio*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 762 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Brometo de ipratrópio*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Brometo de ipratrópio	15C04-B02-321674	22747	40
Fagron	Brometo de ipratrópio	16K07-B05-335330	23597	40
Fagron	Brometo de ipratrópio	18B19-B05-346997	23992	40
Fagron	Brometo de ipratrópio	21E27-B06-213614	25903SI†	10
Fagron	Brometo de ipratrópio	23C07-B08-230203	26897SI†	20

- 201 934 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 15 *Apo-Ident* customers from 13 batches from the substance/substance group *Brometo de ipratrópio*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Brometo de ipratrópio	21E27-B06-213614	1
Euro OTC	Brometo de ipratrópio	18B19-B05-348556	1
Fagron	Brometo de ipratrópio	14B05-B16-294566	1
Fagron	Brometo de ipratrópio	15C04-B02-321674	1
Fagron	Brometo de ipratrópio	18B19-B05-348556	2
Fagron	Brometo de ipratrópio	18B19-B05-356276	8
Fagron	Brometo de ipratrópio	18H30-B09-359170	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Brometo de ipratrópio	18H30-B09-367187/1850002262	1
Fagron	Brometo de ipratrópio	21A14-F02	2
Fagron	Brometo de ipratrópio	21A14-F02377074	1
Fagron	Brometo de ipratrópio	21A14-F02-377075	2
Fagron	Brometo de ipratrópio	21E27-B06-213614	3
Fagron	Brometo de ipratrópio	F02-3770705	1
Fargon	Brometo de ipratrópio	18B19-B055-356276	1
Fragon	Brometo de ipratrópio	2050002969	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Brometo de ipratrópio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Brometo de ipratrópio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	150	0	201 934
Type C	0	27	0	236 040

The substance/substance group *Brometo de ipratrópio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20911	20911	0,00	189,46
21272	20911	7,81	189,88
24947	20911	16,98	193,18
25903	20911	23,60	191,78
26897	20911	15,46	188,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Brometo de neostigmina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20717-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Brometo de neostigmina; Neostigmina, brometo; Neostigmini bromidum

Special notes

When selecting the *Brometo de neostigmina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Brometo de neostigmina	5	3	12

Second-stage model

For differentiation of the substance/substance group *Brometo de neostigmina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Brometo de neostigmina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloreto de dequalínio	113,63	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Brometo de neostigmina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Brometo de neostigmina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Brometo de neostigmina	10144105	20717	40	20100616
Caelo	Brometo de neostigmina	12172304	20990	40	1403163
Caelo	Brometo de neostigmina	14256802	21816	60	AR-15-FG-014460-01
Caelo	Brometo de neostigmina	14256802	21816SI	60	AR-15-FG-014460-01
Caelo	Brometo de neostigmina	15228101	21919	60	20151002
Caelo	Brometo de neostigmina	15228101	21919SI	60	20151002
Caelo	Brometo de neostigmina	193083001	25390	40	20191213

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 7 reference samples from the substance/substance group *Brometo de neostigmina*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 602 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 7 reference samples from the substance/substance group *Brometo de neostigmina*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Brometo de neostigmina	171319	23369	40
Caelo	Brometo de neostigmina	17131901	23373	40
Caelo	Brometo de neostigmina	22000195	26012	40
Caelo	Brometo de neostigmina	171319	23369SI	40
Caelo	Brometo de neostigmina	17131901	23373SI	40
Caelo	Brometo de neostigmina	193083001	25390SI†	40
Caelo	Brometo de neostigmina	22000195	26012SI	40

- 201 804 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 43 spectra from 18 *Apo-Ident* customers from 16 batches from the substance/substance group *Brometo de neostigmina*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Brometo de neostigmina	12172301	1
Caelo	Brometo de neostigmina	12172304	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Brometo de neostigmina	13177201	1
Caelo	Brometo de neostigmina	13177203	2
Caelo	Brometo de neostigmina	13177206	6
Caelo	Brometo de neostigmina	131772303A	1
Caelo	Brometo de neostigmina	131772303B	1
Caelo	Brometo de neostigmina	14256802	3
Caelo	Brometo de neostigmina	15228101	3
Caelo	Brometo de neostigmina	15228103	2
Caelo	Brometo de neostigmina	17131901	4
Caelo	Brometo de neostigmina	17131903	5
Caelo	Brometo de neostigmina	18024902	2
Caelo	Brometo de neostigmina	193083001	3
Caelo	Brometo de neostigmina	20003839001	1
Caesar & Loretz GmbH	Brometo de neostigmina	18024902	2
Gehe	Brometo de neostigmina	12172301	1
Gehe	Brometo de neostigmina	12172307	1
Gehe	Brometo de neostigmina	13177201	1
Hetterich/Noewda	Brometo de neostigmina	17131901	1
Sanacorp	Brometo de neostigmina	18024902	1

- 236 024 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Brometo de neostigmina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Brometo de neostigmina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	280	0	201 804
Type C	0	43	0	236 024

The substance/substance group *Brometo de neostigmina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.0465 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20717	20990	7,00	154,76
20990	20990	0,00	156,82
21816	21816	0,00	185,85
21919	21816	28,00	174,28
25390	20990	37,69	167,62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bromidrato de dextrometorfano**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22318-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bromidrato de dextrometorfano; Dextromethorphani hydrobromidum monohydricum; Dextrometorfano bromidrato

Special notes

When selecting the *Bromidrato de dextrometorfano* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bromidrato de dextrometorfano	7	3	7

Second-stage model

For differentiation of the substance/substance group *Bromidrato de dextrometorfano* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bromidrato de dextrometorfano* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	101,80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bromidrato de dextrometorfano* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bromidrato de dextrometorfano*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bromidrato de dextrometorfano	15D23-B07-308849	22318	60	AR-16-FG-008487-02
Fagron	Bromidrato de dextrometorfano	15D23-B07-308849	22326	60	20150508
Fagron	Bromidrato de dextrometorfano	16A22-B03-321371	23103	40	20160205
Fagron	Bromidrato de dextrometorfano	17B28-B01-341594	23780	40	20170612
Fagron	Bromidrato de dextrometorfano	19A08-B03-363561	24949	40	20190201
Fagron	Bromidrato de dextrometorfano	21F02-B05-221069	26283	40	20210909
Fagron	Bromidrato de dextrometorfano	21F02-B05-221069	26283SI	20	20210909
Fagron	Bromidrato de dextrometorfano	23A21-B02-225362	26633	40	20230222
Fagron	Bromidrato de dextrometorfano	23E30-B01-230367	26817	40	20230616
Fagron	Bromidrato de dextrometorfano	23E30-B01-230367	26817SI	20	20230616

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Bromidrato de dextrometorfano*. These samples are listed above in the *calibration samples* section. The reference

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

samples come from 7 different batches.

- 152 562 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Bromidrato de dextrometorfano*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Bromidrato de dextrometorfano	16E23-B02-329706	23593	40
Fagron	Bromidrato de dextrometorfano	18B09-B02-350261	24288	40
Fagron	Bromidrato de dextrometorfano	23L12-B03-234621	27166	40
Fagron	Bromidrato de dextrometorfano	23A21-B02-225362	26633SI†	20

- 201 944 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 8 *Apo-Ident* customers from 9 batches from the substance/substance group *Bromidrato de dextrometorfano*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Bromidrato de dextrometorfano	17B28-B01-345398	1
Fagron	Bromidrato de dextrometorfano	14H27-B04-299502	7

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bromidrato de dextrometorfano	16A22-B03-319331	1
Fagron	Bromidrato de dextrometorfano	16A22-B03-321371	5
Fagron	Bromidrato de dextrometorfano	18809-B02-358862	1
Fagron	Bromidrato de dextrometorfano	18B09-B02-350261	1
Fagron	Bromidrato de dextrometorfano	18B09-B02-358862	1
Fagron	Bromidrato de dextrometorfano	19A08-B03-363561	1
Phoenix	Bromidrato de dextrometorfano	19A08-B03-363562	1

- 236 048 spectra from 1515 *Apo-Ident* customers from a total of 49 250 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bromidrato de dextrometorfano* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bromidrato de dextrometorfano* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	140	0	201 944
Type C	0	19	0	236 048

The substance/substance group *Bromidrato de dextrometorfano* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22318	22318	0,00	129,25
22326	22318	4,44	129,01
23103	22318	6,93	129,41
23780	22318	10,86	129,65
24949	22318	13,66	131,36
26283	22318	10,20	129,73
26633	22318	12,64	130,29
26817	22318	14,41	129,96

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bromidrato de hioscina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21676-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bromidrato de hioscina; Hioscina, bromidrato; Scopolamini hydrobromidum

Special notes

When selecting the *Bromidrato de hioscina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bromidrato de hioscina	7	3	28

Second-stage model

For differentiation of the substance/substance group *Bromidrato de hioscina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bromidrato de hioscina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	78,09	–
⋮	⋮	⋮
Riboflavina	>50	57,82
Tosilcloramida sódica	>50	69,01
Sulfato de polimixina B	>50	71,00
Bacitracina	>50	86,91
Sulfato de colistina	>50	90,05
Cianocobalamina	>50	95,64
Anfotericina B	>50	126,25
Pantotenato de cálcio	>50	139,48
Triancinolona	>50	145,90
Estriol	>50	151,58
Estradiol hemi-hidratado	>50	158,98
Nistatina	>50	168,80
Vitamina E acetato pó 50%	>50	188,51
Glicerofosfato de cálcio	>50	207,79
Metilcobalamina	>50	216,14
SyrSpend® SF pH4 neo	>50	232,83
Ácido oxálico	>50	250,88
SyrSpend® SF Alka	>50	267,51
Gelatina, branca	>50	277,11
Levedura de selênio	>50	284,21
Amido de arroz	>50	312,06
Carmelose sódica	>50	360,42
Amido de trigo	>50	394,99
SyrSpend® SF pH4	>50	470,03
Fécula de batata	>50	487,35
Frutose	>50	519,47
Amido de milho	>50	529,02
Goma arábica, dispersão seca	>50	536,12
Maltodextrina	>50	637,18

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bromidrato de hioscina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bromidrato de hioscina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bromidrato de hioscina	14278801	21676	60	1504154
Caelo	Bromidrato de hioscina	15054501	21764	60	1511156
Caelo	Bromidrato de hioscina	15054501	21764SI	28	1511156
Caelo	Bromidrato de hioscina	190869	24880	40	20190604*
Caelo	Bromidrato de hioscina	190869	24880SI	40	20190604*
Caelo	Bromidrato de hioscina	172303	24881	40	20170926*
Caelo	Bromidrato de hioscina	21001472001	25733	40	20210423
Caelo	Bromidrato de hioscina	21001472001	25733SI	40	20210423
Fagron	Bromidrato de hioscina	15L09-B04-334706	23418	40	20151228
Fagron	Bromidrato de hioscina	15L09-B04-334706	23418SI	40	20151228
Fagron	Bromidrato de hioscina	15L09-B04-334706	23419	40	20151228
Fagron	Bromidrato de hioscina	15L09-B04-334706	23419SI	40	20151228
Fagron	Bromidrato de hioscina	19G29-B02-367045	25042	40	20191223

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 548 spectra of 13 reference samples from the substance/substance group *Bromidrato de hioscina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 414 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 442 spectra of 11 reference samples from the substance/substance group *Bromidrato de hioscina*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bromidrato de hioscina	15054504	21925	60
Caelo	Bromidrato de hioscina	22003532001	26474	40
Fagron	Bromidrato de hioscina	21G10-B13-221851	26323	40
Caelo	Bromidrato de hioscina	15054501	21764SI†	32
Caelo	Bromidrato de hioscina	15054504	21925SI	30
Caelo	Bromidrato de hioscina	15054504	23441	40
Caelo	Bromidrato de hioscina	15054504	23441SI	40
Caelo	Bromidrato de hioscina	172303	24881SI†	40
Caelo	Bromidrato de hioscina	22003532001	26474SI	40
Fagron	Bromidrato de hioscina	19G29-B02-367045	25042SI†	40
Fagron	Bromidrato de hioscina	21G10-B13-221851	26323SI	40

- 201 642 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 75 spectra from 33 *Apo-Ident* customers from 30 batches from the substance/substance group *Bromidrato de hioscina*.
- Among them are spectra of independent samples from 28 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bromidrato de hioscina	22003532001	1
	Bromidrato de hioscina	22003532004	2
Caelo	Bromidrato de hioscina	14278801	26
Caelo	Bromidrato de hioscina	15054505	1
Caelo	Bromidrato de hioscina	15054511	1
Caelo	Bromidrato de hioscina	15358901	1
Caelo	Bromidrato de hioscina	16206204	1
Caelo	Bromidrato de hioscina	16206208	1
Caelo	Bromidrato de hioscina	17230303	2
Caelo	Bromidrato de hioscina	18024806	4
Caelo	Bromidrato de hioscina	18024807	4
Caelo	Bromidrato de hioscina	190869002	1
Caelo	Bromidrato de hioscina	19086901	5
Caelo	Bromidrato de hioscina	20001949001	4
Caelo	Bromidrato de hioscina	21000424002	1
Caesar & Loretz GmbH	Bromidrato de hioscina	20001949001	1
Caesar & Loretz GmbH	Bromidrato de hioscina	21001472001	1
Caesar & Loretz GmbH	Bromidrato de hioscina	22000116002	1
Fagron	Bromidrato de hioscina	14F11-B02-296840	1
Fagron	Bromidrato de hioscina	14J27-B05-307020	2
Fagron	Bromidrato de hioscina	15L09-B04-327494	1
Fagron	Bromidrato de hioscina	17D18-B05-335528	2
Fagron	Bromidrato de hioscina	18B23-B04-357420	1
Fagron	Bromidrato de hioscina	19G29-B02	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bromidrato de hioscina	21G28-F04	1
Fagron	Bromidrato de hioscina	21G28-F04-379942	1
Fagron	Bromidrato de hioscina	21G28-F04-379944	2
Fagron	Bromidrato de hioscina	2630421	1
Fagron	Bromidrato de hioscina	B02-3670405	1
Gehe	Bromidrato de hioscina	19086901	1
Phönix	Bromidrato de hioscina	19869002	1
Sanacorp	Bromidrato de hioscina	2100424002	1

- 235 992 spectra from 1515 *Apo-Ident* customers from a total of 49 228 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bromidrato de hioscina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bromidrato de hioscina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	548	0	152 414
Type B	0	442	0	201 642
Type C	0	75	0	235 992

The substance/substance group *Bromidrato de hioscina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9051 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6425 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21676	21676	0,00	94,08
21764	21764	0,00	87,00
23418	21764	44,31	127,76
23419	21764	45,98	133,52
24880	24880	0,00	94,65
24881	24881	0,00	71,70
25042	21676	7,53	96,36
25733	21764	28,18	89,06

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bromidrato de homatropina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24442-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bromidrato de homatropina; Homatropini hydrobromidum; Homotropina, bromidrato

Special notes

When selecting the *Bromidrato de homatropina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bromidrato de homatropina	2	2	0

Second-stage model

For differentiation of the substance/substance group *Bromidrato de homatropina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bromidrato de homatropina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	120,04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bromidrato de homatropina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bromidrato de homatropina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bromidrato de homatropina	18L11-B03-356938	24442	40	1905511
Fagron	Bromidrato de homatropina	23G12-B16-233048	27020	40	20230726
Fagron	Bromidrato de homatropina	23G12-B16-233048	27020SI	20	20230726

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Bromidrato de homatropina*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 862 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 4 reference samples from the substance/substance group *Bromidrato de homatropina*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Bromidrato de homatropina	21J07-B04-213599	26056	40
Fagron	Bromidrato de homatropina	24D24-B09-000930	27375	40
Fagron	Bromidrato de homatropina	21J07-B04-213599	26056SI	20
Fagron	Bromidrato de homatropina	24D24-B09-000930	27375SI	20

- 201 964 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Bromidrato de homatropina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bromidrato de homatropina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bromidrato de homatropina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	120	0	201 964
Type C	0	0	0	236 067

The substance/substance group *Bromidrato de homatropina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24442	24442	0,00	185,05
27020	24442	7,75	182,27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Budesonida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20569-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Budesonida; Budesonidum

Special notes

When selecting the *Budesonida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Budesonida	8	13	186

Second-stage model

For differentiation of the substance/substance group *Budesonida* the following second-stage model is used:

- Submodelo 07

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Budesonida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	72,92	–
⋮	⋮	⋮
Valerato de betametasona	>50	20,70
Eritromicina	>50	34,26

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Budesonida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Budesonida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Budesonida	11351704	20808	40	AR-15-FG-005286-01
Caelo	Budesonida	161431	22627	40	20160606*
Caelo	Budesonida	161431	22627SI	25	20160606*
Caelo	Budesonida	15344004	22649	40	20151116
Caelo	Budesonida	15344004	22649SI	23	20151116
Euro OTC	Budesonida	1311022-01	21620	60	20140113
Euro OTC	Budesonida	1311022-01	21620SI	37	20140113
Euro OTC	Budesonida	1604018	22537	40	20160509*
Euro OTC	Budesonida	1604018	22537SI	23	20160509*
Euro OTC	Budesonida	2010006	25475	40	20201202*
Fagron	Budesonida	16J04-B01-326581	22841	40	20161026
Fagron	Budesonida	16J04-B01-326581	22888	40	20161026
Fagron	Budesonida	16J04-B01-326581	22888SI	30	20161026
Fagron	Budesonida	18C15-B03-355399	24699	40	20180409

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 518 spectra of 14 reference samples from the substance/substance group *Budesonida*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 444 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1021 spectra of 30 reference samples from the substance/substance group *Budesonida*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Budesonida	170788	23279	40
Caelo	Budesonida	180749	24026	40
Caelo	Budesonida	191381	24737	40
Caelo	Budesonida	20002391	25636	30
Caelo	Budesonida	23000636	26710	40
Euro OTC	Budesonida	1709022	23778	40
Euro OTC	Budesonida	1904004	24619	40
Euro OTC	Budesonida	2003043	25251	40
Euro OTC	Budesonida	2103025	25690	50
Euro OTC	Budesonida	2203005	26088	40
Euro OTC	Budesonida	2301044	26590	30
Euro OTC	Budesonida	2402017	27150	40
Fagron	Budesonida	22A12-B01-213702	26378	40
Caelo	Budesonida	15344004	22649SI†	7
Caelo	Budesonida	170788	23279SI	20
Caelo	Budesonida	180749	24026SI	20
Caelo	Budesonida	191381	24737SI	24
Caelo	Budesonida	20002391	25636SI	30
Caelo	Budesonida	23000636	26710SI	30
Euro OTC	Budesonida	1709022	23778SI	20

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Budesonida	1904004	24619SI	40
Euro OTC	Budesonida	2003043	25251SI	40
Euro OTC	Budesonida	2010006	25475SI†	39
Euro OTC	Budesonida	2103025	25690SI	50
Euro OTC	Budesonida	2203005	26088SI	40
Euro OTC	Budesonida	2301044	26590SI	32
Euro OTC	Budesonida	2402017	27150SI	30
Fagron	Budesonida	16J04-B01-326581	22841SI†	24
Fagron	Budesonida	18C15-B03-355399	24699SI†	35
Fagron	Budesonida	22A12-B01-213702	26378SI	30

- 201 063 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 869 spectra from 256 *Apo-Ident* customers from 194 batches from the substance/substance group *Budesonida*.
- Among them are spectra of independent samples from 186 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Budesonida	20004092009	1
	Budesonida	20004092016	1
	Budesonida	20004092018	1
	Budesonida	20004092024	2
	Budesonida	20004092026	3
	Budesonida	21I20-B03-215349	1
	Budesonida	22A12-B01-228674	1
	Budesonida	23000636001	3
	Budesonida	23000636003	7
	Budesonida	23000636009	1
	Budesonida	23000636010	1
Anzag	Budesonida	19138101	1
Anzag	Budesonida	19138102	2
Bombastus	Budesonida	21100M1A0021321	1
Caelo	Budesonida	10061705	1
Caelo	Budesonida	11175014	2
Caelo	Budesonida	11175015	1
Caelo	Budesonida	11351701	1
Caelo	Budesonida	11351703	1
Caelo	Budesonida	11351706	5
Caelo	Budesonida	11351707	3
Caelo	Budesonida	11351713	1
Caelo	Budesonida	12295103	1
Caelo	Budesonida	12295105	1
Caelo	Budesonida	12295106	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Budesonida	12295108	1
Caelo	Budesonida	12295109	2
Caelo	Budesonida	12295110	4
Caelo	Budesonida	12295111	5
Caelo	Budesonida	1407116	1
Caelo	Budesonida	140711707	1
Caelo	Budesonida	14071701	2
Caelo	Budesonida	14071702	6
Caelo	Budesonida	14071706	1
Caelo	Budesonida	14071707	4
Caelo	Budesonida	14071713	1
Caelo	Budesonida	14071714	6
Caelo	Budesonida	14071716	2
Caelo	Budesonida	14071717	3
Caelo	Budesonida	1471707	1
Caelo	Budesonida	15044002	1
Caelo	Budesonida	15173802	4
Caelo	Budesonida	15173803	6
Caelo	Budesonida	15173804	3
Caelo	Budesonida	15173806	4
Caelo	Budesonida	15173807	3
Caelo	Budesonida	15173810	1
Caelo	Budesonida	15173811	8
Caelo	Budesonida	15344002	4
Caelo	Budesonida	15344003	7
Caelo	Budesonida	15344004	1
Caelo	Budesonida	15344005	4
Caelo	Budesonida	15344006	4
Caelo	Budesonida	15344008	8
Caelo	Budesonida	15344009	2
Caelo	Budesonida	15344010	3
Caelo	Budesonida	15344012	4
Caelo	Budesonida	15344013	1
Caelo	Budesonida	15344014	1
Caelo	Budesonida	16143101	7
Caelo	Budesonida	16143102	2
Caelo	Budesonida	16143103	3
Caelo	Budesonida	16143105	2
Caelo	Budesonida	16143106	3
Caelo	Budesonida	16143107	5
Caelo	Budesonida	16143108	10
Caelo	Budesonida	16143110	2
Caelo	Budesonida	16143112	2
Caelo	Budesonida	170078801	1
Caelo	Budesonida	170078808	1
Caelo	Budesonida	17078801	17
Caelo	Budesonida	17078803	3
Caelo	Budesonida	17078804	7
Caelo	Budesonida	17078805	16
Caelo	Budesonida	17078808	9
Caelo	Budesonida	17078809	6
Caelo	Budesonida	1709022	1
Caelo	Budesonida	17342902	5
Caelo	Budesonida	18074901	5
Caelo	Budesonida	18074902	11
Caelo	Budesonida	18074903	11
Caelo	Budesonida	18074905	11
Caelo	Budesonida	18074907	10
Caelo	Budesonida	18074908	11
Caelo	Budesonida	18074909	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Budesonida	181720608	1
Caelo	Budesonida	18172601	3
Caelo	Budesonida	18172603	14
Caelo	Budesonida	18172604	19
Caelo	Budesonida	18172606	6
Caelo	Budesonida	18172607	13
Caelo	Budesonida	18172608	8
Caelo	Budesonida	18172609	5
Caelo	Budesonida	18172610	3
Caelo	Budesonida	18172611	11
Caelo	Budesonida	18172614	4
Caelo	Budesonida	191381002	3
Caelo	Budesonida	191381004	13
Caelo	Budesonida	191381005	2
Caelo	Budesonida	19138101	22
Caelo	Budesonida	19138101P-200511-1	1
Caelo	Budesonida	19138101P-200709-1	1
Caelo	Budesonida	19138101P-200727-2	1
Caelo	Budesonida	19138102	27
Caelo	Budesonida	19138103	10
Caelo	Budesonida	200004092007	1
Caelo	Budesonida	200004092016	1
Caelo	Budesonida	20001092012	1
Caelo	Budesonida	2000402008	2
Caelo	Budesonida	20004092001	4
Caelo	Budesonida	20004092002	2
Caelo	Budesonida	20004092003	6
Caelo	Budesonida	20004092005	7
Caelo	Budesonida	20004092006	5
Caelo	Budesonida	20004092007	11
Caelo	Budesonida	20004092008	4
Caelo	Budesonida	20004092009	9
Caelo	Budesonida	20004092011	5
Caelo	Budesonida	20004092012	2
Caelo	Budesonida	20004092013	3
Caelo	Budesonida	20004092014	1
Caelo	Budesonida	20004092015	5
Caelo	Budesonida	20004092016	1
Caelo	Budesonida	20004092017	1
Caelo	Budesonida	20004092018	2
Caelo	Budesonida	20004092019	1
Caelo	Budesonida	20004092022	6
Caelo	Budesonida	20004092023	2
Caelo	Budesonida	20004092024	1
Caelo	Budesonida	20004092026	3
Caelo	Budesonida	20004092028	1
Caelo	Budesonida	20i17-f07-374500	1
Caelo	Budesonida	21100M1	1
Caelo	Budesonida	23000636003	1
Caelo	Budesonida	774865	1
Caelo	Budesonida	B-240619-2	1
Caelo	Budesonida	ChB14071717	1
Caeolo ,	Budesonida	17078809	1
Caesar & Lorenz GmbH	Budesonida	18172607	1
Caesar & Loretz GmbH...	Budesonida	191381002	1
Caesar & Loretz GmbH...	Budesonida	20004092002	1
Caesar & Loretz GmbH...	Budesonida	19138102	2
Caesar & Loretz GmbH...	Budesonida	19138101	1
Caesar & Loretz GmbH...	Budesonida	19138102	1
Caesar & Loretz GmbH...	Budesonida	20004092003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Budesonida	20004092018	1
Caesar & Loretz GmbH/Gehe	Budesonida	18172607	1
Caesar & Loretz GmbH/Gehe	Budesonida	20004092001	1
Caesar & Loretz GmbH/Gehe	Budesonida	20004092003	1
Caesar & Loretz GmbH/Gehe	Budesonida	20004092008	2
Caesar & Loretz GmbH/Gehe	Budesonida	20004092009	1
Caesar & Loretz GmbH/Gehe	Budesonida	20004092014	1
Caesar & Loretz GmbH...	Budesonida	191381002	1
Caesar & Loretz GmbH...	Budesonida	19138102	1
Caesar & Loretz GmbH...	Budesonida	20004092003	1
Caesar & Loretz GmbH...	Budesonida	20004092006	1
Caesar & Loretz GmbH...	Budesonida	19138102	1
Caesar & Loretz GmbH...	Budesonida	18172606	1
Caesar & Loretz GmbH/Sana	Budesonida	18172610	1
Caesar & Loretz GmbH...	Budesonida	18172603	1
Caesar & Loretz GmbH...	Budesonida	20004092009	1
Caesar & Loretz GmbH	Budesonida	17078808	1
Caesar & Loretz GmbH	Budesonida	17342902	1
Caesar & Loretz GmbH	Budesonida	18074905	1
Caesar & Loretz GmbH	Budesonida	18172603	1
Caesar & Loretz GmbH	Budesonida	18172604	2
Caesar & Loretz GmbH	Budesonida	18172606	5
Caesar & Loretz GmbH	Budesonida	18172608	6
Caesar & Loretz GmbH	Budesonida	18172610	1
Caesar & Loretz GmbH	Budesonida	18172611	3
Caesar & Loretz GmbH	Budesonida	18172614	2
Caesar & Loretz GmbH	Budesonida	1913810	1
Caesar & Loretz GmbH	Budesonida	191381002	8
Caesar & Loretz GmbH	Budesonida	191381004	3
Caesar & Loretz GmbH	Budesonida	191381005	3
Caesar & Loretz GmbH	Budesonida	19138101	11
Caesar & Loretz GmbH	Budesonida	19138102	12
Caesar & Loretz GmbH	Budesonida	19138103	8
Caesar & Loretz GmbH	Budesonida	2000402007	1
Caesar & Loretz GmbH	Budesonida	20004092001	1
Caesar & Loretz GmbH	Budesonida	20004092002	5
Caesar & Loretz GmbH	Budesonida	20004092003	2
Caesar & Loretz GmbH	Budesonida	20004092005	2
Caesar & Loretz GmbH	Budesonida	20004092006	2
Caesar & Loretz GmbH	Budesonida	20004092007	7
Caesar & Loretz GmbH	Budesonida	20004092008	4
Caesar & Loretz GmbH	Budesonida	20004092011	2
Caesar & Loretz GmbH	Budesonida	20004092012	3
Caesar & Loretz GmbH	Budesonida	20004092013	1
Caesar & Loretz GmbH	Budesonida	20004092015	2
Caesar & Loretz GmbH	Budesonida	20004092017	3
Caesar & Loretz GmbH	Budesonida	20004092018	3
Caesar & Loretz GmbH	Budesonida	20004092019	1
Caesar & Loretz GmbH	Budesonida	20004092022	1
Caesar & Loretz GmbH	Budesonida	20004092024	3
Cealo / Otto Geilenk...	Budesonida	19138101	1
Cealo/Gehe	Budesonida	19138103	1
Cealo/Sanacorp	Budesonida	20004092006	1
Cealo	Budesonida	17078804	1
Ceolo/Spangro	Budesonida	191381002	1
crystal pharma/gehe	Budesonida	1305004-01	2
Euro OTC	Budesonida	1311022-01	5
Euro OTC	Budesonida	1604018-01	2
Euro OTC	Budesonida	1709022-01	2
Euro OTC	Budesonida	1709022-02	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Budesonida	18172609	1
Euro OTC	Budesonida	1904004-01	2
Euro OTC	Budesonida	2203005-01	1
Euro OTC	Budesonida	709022-02	1
Fagron	Budesonida		2
Fagron	Budesonida	12D03-N03	1
Fagron	Budesonida	12G23-N01	2
Fagron	Budesonida	13A07-N09	1
Fagron	Budesonida	13H22-N03	2
Fagron	Budesonida	14A30-B09_291366	1
Fagron	Budesonida	14A30-B09-291366	2
Fagron	Budesonida	14H15-B02	3
Fagron	Budesonida	14H15-B02-297926	1
Fagron	Budesonida	14H15-B02-301971	2
Fagron	Budesonida	14H15-B02-301972	1
Fagron	Budesonida	15344012	1
Fagron	Budesonida	15E27_B10	1
Fagron	Budesonida	15E27-B01-308321	1
Fagron	Budesonida	15e27-b10-308321	1
Fagron	Budesonida	15E27-B10-308321	1
Fagron	Budesonida	15e27-b10-308322	1
Fagron	Budesonida	15E27-B10-308322	1
Fagron	Budesonida	15E27-B10-315704	1
Fagron	Budesonida	16J04-B01	1
Fagron	Budesonida	16j04-b01-326583	3
Fagron	Budesonida	17a17-b01	1
Fagron	Budesonida	17A17-B01	1
Fagron	Budesonida	17A17-B01-331248	1
Fagron	Budesonida	17A17-B01-331448	4
Fagron	Budesonida	17F28-B04-345016	2
Fagron	Budesonida	18074901	1
Fagron	Budesonida	18172601	1
Fagron	Budesonida	18C15-B03-350266	4
Fagron	Budesonida	18C15-B03-353058	2
Fagron	Budesonida	18C15-B03-355399	3
Fagron	Budesonida	19/27-F02-366343	1
Fagron	Budesonida	19F06-B06	2
Fagron	Budesonida	19f06-B06-363444	1
Fagron	Budesonida	19F06-B06-363447	1
Fagron	Budesonida	19F-06-B06-363447	1
Fagron	Budesonida	19I27-F02-366344	1
Fagron	Budesonida	1B001192001	1
Fagron	Budesonida	1B00119201	1
Fagron	Budesonida	1B003202001	2
Fagron	Budesonida	20/17-F07	1
Fagron	Budesonida	20G17-F03-372894	1
Fagron	Budesonida	20G17-F03-372894	1
Fagron	Budesonida	20I17-F07	1
Fagron	Budesonida	20I17-F07-374499	2
Fagron	Budesonida	20l17-F07-374500	1
Fagron	Budesonida	21b05_b17-213703	1
Fagron	Budesonida	21B05-B17	1
Fagron	Budesonida	21I20-B03-215348	1
Fagron	Budesonida	21I20-B03-215664	1
Fagron	Budesonida	21l20-B03-215664	1
Fagron	Budesonida	C2280092	1
Fargon/Kehr	Budesonida	16J04-B01-326583	1
Farmabios/Noweda	Budesonida	21100M1B0031821	2
Farmabios/Phoenix	Budesonida	21100M1B0021821	1
Gehe	Budesonida	14071714	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Budesonida	16143103	1
Gehe	Budesonida	16143107	1
Gehe	Budesonida	17078801	1
GEHE	Budesonida	18074901	1
Gehe	Budesonida	18074902	3
GEHE	Budesonida	18172601	2
Gehe	Budesonida	18172604	1
Gehe	Budesonida	20004092024	1
Geibo/ Fargron	Budesonida	15E27-B10-315704	1
Geibo/ Fargron	Budesonida	17A17-b01-331448	1
Jenne	Budesonida	20004092024	1
L10	Budesonida	15344012	1
Noweda/Caesar & Lore...	Budesonida	19138101	1
Noweda	Budesonida	1604018-01	1
Noweda	Budesonida	16143108	1
Noweda	Budesonida	16143110	1
Noweda	Budesonida	17078803	1
Noweda	Budesonida	18074903	1
Noweda	Budesonida	18172608	1
Noweda	Budesonida	191381004	1
Noweda	Budesonida	20004092012	1
Noweda	Budesonida	20004092022	1
Noweda	Budesonida	20004092028	1
Noweda	Budesonida	23000636001	2
Otto Geilenkirchen	Budesonida	23000636003	1
Phoenix	Budesonida	14071702	3
Phoenix	Budesonida	15344013	1
phoenix	Budesonida	19138103	1
Phoenix	Budesonida	23000636009	1
Phönix	Budesonida	18074907	1
Phönix	Budesonida	18172607	1
Phönix	Budesonida	191381004	1
Sanacorp /Fargron	Budesonida	17A17-B01-331448	1
Sanacorp,	Budesonida	16143103	1
sanacorp	Budesonida	14071701	1
Sanacorp	Budesonida	17078801	1
Sanacorp	Budesonida	17078805	1
Sanacorp	Budesonida	18074902	1
Sanacorp	Budesonida	18074907	1
sanacorp	Budesonida	191381004	1
Sanacorp	Budesonida	20004092024	1
Sanacorp	Budesonida	20004092029	1
Sanacorp	Budesonida	23000636003	1
Sanacorp	Budesonida	23000636004	1
VDl 23.10.14 19,50 euro	Budesonida	14071707	1

- 235 198 spectra from 1515 *Apo-Ident* customers from a total of 49 068 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Budesonida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Budesonida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table

breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	518	0	152 444
Type B	0	1021	0	201 063
Type C	0	820	49	235 198

The substance/substance group *Budesonida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8417 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4123 %)
Type C	100.0000 % (> 99.9007 %)	94.3613 % (> 94.0161 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20808	20808	0,00	139,72
21620	20808	5,23	131,19
22537	22537	0,00	116,23
22627	22627	0,00	121,71
22649	22537	7,87	119,24
22841	22627	4,41	122,54
22888	22627	7,99	122,90
24699	25475	8,11	120,73
25475	25475	0,00	124,81

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cafeína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20962-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cafeína; Coffeinum

Special notes

When selecting the *Cafeína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cafeína	7	9	100

Second-stage model

For differentiation of the substance/substance group *Cafeína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cafeína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citrato de cafeína	142,24	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cafeína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cafeína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cafeína	12317911	21089	40	20121113
Caelo	Cafeína	12317911	21205	40	20121113
Caelo	Cafeína	13233105	21456	60	20131008
Caelo	Cafeína	13233104	21548	60	20131008
Euro OTC	Cafeína	1211012-01	20962	40	1412248
Euro OTC	Cafeína	1808017	24199	40	20180905*
Euro OTC	Cafeína	1909022	24980	40	20191022*
Fagron	Cafeína	22A19-B05-219102	26161	40	20220531

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 360 spectra of 8 reference samples from the substance/substance group *Cafeína*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 12 reference samples from the substance/substance group *Cafeína*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cafeína	15082303	22823	40
Caelo	Cafeína	21001749	25798	50
Caelo	Cafeína	23000642	26711	40
Euro OTC	Cafeína	1603009	22517	40
Euro OTC	Cafeína	1703006	23140	40
Euro OTC	Cafeína	1907006	24784	40
Euro OTC	Cafeína	2001041	25079	40
Euro OTC	Cafeína	2205020	26201	40
Euro OTC	Cafeína	2311014	27068	40
Caelo	Cafeína	23000642	26711SI	20
Euro OTC	Cafeína	2205020	26201SI	20
Fagron	Cafeína	22A19-B05-219102	26161SI†	20

- 201 654 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 470 spectra from 271 *Apo-Ident* customers from 105 batches from the substance/substance group *Cafeína*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 99 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cafeína	20014041-02	1
	Cafeína	21052089	1
	Cafeína	22002096001	3
	Cafeína	22002096010	2
	Cafeína	2205020-01	1
	Cafeína	2205020-02	2
	Cafeína	2205020-03	4
	Cafeína	2205050-03	1
	Cafeína	23000642003	2
	Cafeína	2311014-01	2
ACM	Cafeína	KNC1294J14	2
AHD	Cafeína	2205020-03	1
Alliance Healthcare	Cafeína	18011928	1
apo-ident	Cafeína	1808017-01	1
Bombastus	Cafeína	1307049-01	1
Caelo	Cafeína	11076807	2
Caelo	Cafeína	11111111	1
Caelo	Cafeína	12093402	2
Caelo	Cafeína	12093410	2
Caelo	Cafeína	12093418	2
Caelo	Cafeína	1211012-01	1
Caelo	Cafeína	12317902	1
Caelo	Cafeína	12317904	2
Caelo	Cafeína	12317906	1
Caelo	Cafeína	12317909	8
Caelo	Cafeína	12317914	2
Caelo	Cafeína	13233105	4
Caelo	Cafeína	13233111	6
Caelo	Cafeína	1503020-01	2
Caelo	Cafeína	15054704	3
Caelo	Cafeína	15054709	3
Caelo	Cafeína	15082311	1
Caelo	Cafeína	15082315	1
Caelo	Cafeína	15372012	1
Caelo	Cafeína	15375006	4
Caelo	Cafeína	15375007	6
Caelo	Cafeína	15375012	6
Caelo	Cafeína	15375013	1
Caelo	Cafeína	1703006-01	4
Caelo	Cafeína	17133704	1
Caelo	Cafeína	17173704	10
Caelo	Cafeína	17173705	10
Caelo	Cafeína	17173707	5
Caelo	Cafeína	180119001	1
Caelo	Cafeína	180119002	3
Caelo	Cafeína	18011901	6
Caelo	Cafeína	18011902	6
Caelo	Cafeína	18011906	9
Caelo	Cafeína	18011911	38
Caelo	Cafeína	18011915	9
Caelo	Cafeína	18011920	14
Caelo	Cafeína	18011928	8
Caelo	Cafeína	180119911	1
Caelo	Cafeína	18077906	1
Caelo	Cafeína	1808017-01	1
Caelo	Cafeína	19000754002	13
Caelo	Cafeína	1907006-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cafeína	21000088004	26
Caelo	Cafeína	21000088006	1
Caelo	Cafeína	21001749004	2
Caelo	Cafeína	21001749006	3
Caelo	Cafeína	21001749014	2
Caelo	Cafeína	21001749015	3
Caelo	Cafeína	22002096001	2
Caelo	Cafeína	22002096010	10
Caelo	Cafeína	3212E-01281	1
Caelo	Cafeína	9301807	1
Caesar & Lorenz	Cafeína	22002096001	1
Caesar & Loretz GmbH...	Cafeína	21001749002	1
Caesar & Loretz GmbH...	Cafeína	21001749004	1
Caesar & Loretz GmbH...	Cafeína	19000754002	3
Caesar & Loretz GmbH...	Cafeína	180119002	1
Caesar & Loretz GmbH	Cafeína	180119001	1
Caesar & Loretz GmbH	Cafeína	180119002	3
Caesar & Loretz GmbH	Cafeína	18011912	2
Caesar & Loretz GmbH	Cafeína	18011915	2
Caesar & Loretz GmbH	Cafeína	18011920	2
Caesar & Loretz GmbH	Cafeína	18011928	2
Caesar & Loretz GmbH	Cafeína	19000754002	4
Caesar & Loretz GmbH	Cafeína	21000088004	2
Caesar & Loretz GmbH	Cafeína	21000088006	2
Caesar & Loretz GmbH	Cafeína	21001749002	1
Caesar & Loretz GmbH	Cafeína	21001749004	1
Caesar & Loretz GmbH	Cafeína	21001749006	3
Caesar & Loretz GmbH	Cafeína	21001749014	1
Caesar & Loretz GmbH	Cafeína	21001749015	1
Caesar & Loretz GmbH	Cafeína	22002096001	1
Caesar&Loretz GmbH	Cafeína	21001749006	1
EuRho	Cafeína	17030006-02	2
EuRho	Cafeína	1808017-02	1
Euro OTC	Cafeína		1
Euro OTC	Cafeína	1109017-01	1
Euro OTC	Cafeína	1211012-01	1
Euro OTC	Cafeína	1211012-02	1
Euro OTC	Cafeína	1307049-01	4
Euro OTC	Cafeína	1404026-01	1
Euro OTC	Cafeína	1411015-01	4
Euro OTC	Cafeína	1503020-01	6
Euro OTC	Cafeína	1503020-02	8
Euro OTC	Cafeína	1603009/01	1
Euro OTC	Cafeína	160300901	2
Euro OTC	Cafeína	1603009-01	2
Euro OTC	Cafeína	1603009-02	4
Euro OTC	Cafeína	163009-01	1
Euro OTC	Cafeína	16462119	1
Euro OTC	Cafeína	1703006	1
Euro OTC	Cafeína	1703006-01	23
Euro OTC	Cafeína	1703006-02	9
Euro OTC	Cafeína	17173704	1
Euro OTC	Cafeína	1808017	3
Euro OTC	Cafeína	1808017_01	1
Euro OTC	Cafeína	1808017-01	7
Euro OTC	Cafeína	180801702	1
Euro OTC	Cafeína	1808017-02	3
Euro OTC	Cafeína	180881701	1
Euro OTC	Cafeína	1818017-02	1
Euro OTC	Cafeína	18212023	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cafeína	18808017-01	1
Euro OTC	Cafeína	1907006-01	5
Euro OTC	Cafeína	1907006-1	1
Euro OTC	Cafeína	1909022-01	5
Euro OTC	Cafeína	2001041-01	3
Euro OTC	Cafeína	2001041-02	12
Euro OTC	Cafeína	2205020-01	1
Euro OTC	Cafeína	2205020-02	1
Euro OTC	Cafeína	26081406	1
Euro OTC	Cafeína	291001903	2
Euro OTC	Cafeína	31071701	1
Euro OTC	Cafeína	325241AX20	1
Euro OTC	Cafeína	5101701	1
EUro/AHD	Cafeína	121012-01	1
EUro/AHD	Cafeína	1307049-01	1
Euro/Noweda	Cafeína	1703006-01	1
Fagron	Cafeína	123456	1
Fagron	Cafeína	15H11-B02	1
Fagron	Cafeína	17173704	1
Gatt-Koller / Phoenix	Cafeína	5898/12135213	2
Gatt-Koller	Cafeína	1803747	1
Gehe	Cafeína	18011915	2
GEHE	Cafeína	22002096001	1
Gehe	Cafeína	23000642002	1
Gehe	Cafeína	23000642003	1
Klenk	Cafeína	1411015-01	1
Merck	Cafeína	MerckReagenziensatz	1
Noweda/Caesar & Lore…	Cafeína	21001749014	1
Noweda	Cafeína	1404026-01	1
Noweda	Cafeína	2001041-01	1
Phoenix	Cafeína	1808017-01	1
Phönix	Cafeína	1603009-02	1
Reagenz	Cafeína		1
Sanacorp	Cafeína		2
Sanacorp	Cafeína	19000754002	1
siegfried pharma che…	Cafeína	1909022-01	1
Siegfried PharmaChem…	Cafeína	1808017-01	1

- 235 597 spectra from 1515 *Apo-Ident* customers from a total of 49 156 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cafeína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cafeína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	430	0	201 654
Type C	0	458	12	235 597

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Cafeína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	97.4468 % (> 96.8085 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20962	20962	0,00	232,38
21089	24199	7,15	239,45
21205	24199	6,43	238,47
21456	24980	8,05	236,47
21548	20962	10,42	225,98
24199	24199	0,00	241,53
24980	24980	0,00	246,12
26161	24199	23,57	256,14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Canabidiol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22416-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Canabidiol

Special notes

When selecting the *Canabidiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Canabidiol	7	6	261

Second-stage model

For differentiation of the substance/substance group *Canabidiol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Canabidiol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estriol	98,95	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Canabidiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Canabidiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Canabidiol	21000530	25612	40	20210218*
Caelo	Canabidiol	21000530	25612SI	40	20210218*
Caelo	Canabidiol	21003190	25995	40	20211022*
Caelo	Canabidiol	21003190	25995SI	40	20211022*
THC-Pharma GmbH	Canabidiol	15-7221-80338	22412	60	1316Q-07806
THC-Pharma GmbH	Canabidiol	15-7221-80338	22412SI	60	1316Q-07806
THC-Pharma GmbH	Canabidiol	15-7221-80338	22413	60	1316Q-07806
THC-Pharma GmbH	Canabidiol	15-7221-80338	22414	60	1316Q-07806
THC-Pharma GmbH	Canabidiol	15-7221-80338	22415	60	1316Q-07806
THC-Pharma GmbH	Canabidiol	15-7221-80338	22416	60	1316Q-07806
THC-Pharma GmbH	Canabidiol	CBD-API17-003	23398	40	20170609
THC-Pharma GmbH	Canabidiol	CBD-API17-003	23399	40	20170609
THC-Pharma GmbH	Canabidiol	CBD-API16-003	23464	40	2017B-03911
THC-Pharma GmbH	Canabidiol	CBD-API16-004	23465	40	2017A-03911
THC-Pharma GmbH	Canabidiol	H230.320-1	25504	40	20200806
THC-Pharma GmbH	Canabidiol	H230.320-1	25504SI	40	20200806

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 760 spectra of 16 reference samples from the substance/substance group *Canabidiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 202 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 871 spectra of 20 reference samples from the substance/substance group *Canabidiol*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
ADREXpharma GmbH	Canabidiol	19Y21746	26024	40
Caelo	Canabidiol	21002319	25998	40
Caelo	Canabidiol	22001216	26110	40
Caelo	Canabidiol	23002758005	27193	40
THC-Pharma GmbH	Canabidiol	CBDAPI1801	23929	40
THC-Pharma GmbH	Canabidiol	H150.920-1	25730	40
ADREXpharma GmbH	Canabidiol	19Y21746	26024SI	40
Caelo	Canabidiol	21002319	25998SI	40
Caelo	Canabidiol	22001216	26110SI	40
Caelo	Canabidiol	23002758005	27193SI	40
THC-Pharma GmbH	Canabidiol	15-7221-80338	22413SI†	60
THC-Pharma GmbH	Canabidiol	15-7221-80338	22414SI†	60
THC-Pharma GmbH	Canabidiol	15-7221-80338	22415SI†	60
THC-Pharma GmbH	Canabidiol	15-7221-80338	22416SI†	60
THC-Pharma GmbH	Canabidiol	CBD-API17-003	23398SI†	40
THC-Pharma GmbH	Canabidiol	CBD-API17-003	23399SI†	31
THC-Pharma GmbH	Canabidiol	CBD-API16-003	23464SI†	40
THC-Pharma GmbH	Canabidiol	CBD-API16-004	23465SI†	40
THC-Pharma GmbH	Canabidiol	CBDAPI1801	23929SI	40
THC-Pharma GmbH	Canabidiol	H150.920-1	25730SI	40

- 201 213 spectra from a total of 4035 batches from further 842 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1707 spectra from 179 *Apo-Ident* customers from 290 batches from the substance/substance group *Canabidiol*.
- Among them are spectra of independent samples from 213 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Canabidiol	10C120722-0	1
	Canabidiol	22001216008	3
	Canabidiol	23167A	1
	Canabidiol	23230C	1
	Canabidiol	23231B	1
	Canabidiol	23274B	1
	Canabidiol	23N9251	1
	Canabidiol	ACPN920903	1
	Canabidiol	CA215062024	2
	Canabidiol	CA216062024	1
	Canabidiol	CBD2102A01	1
	Canabidiol	CBD2105A02	1
	Canabidiol	CBDAPI2102	1
	Canabidiol	G23ACV-ICS1	3
	Canabidiol	G23ACV-ICS2	1
	Canabidiol	KI0001	1
	Canabidiol	KI0002	1
	Canabidiol	KI0003	2
	Canabidiol	KI0006	1
	Canabidiol	KI0007	1
	Canabidiol	KI0011	1
	Canabidiol	KI0018	2
	Canabidiol	KI0021	2
	Canabidiol	LL130122022	2
	Canabidiol	LL148032023	6
	Canabidiol	LL164062023	1
	Canabidiol	LL165062023	1
	Canabidiol	LL166062023	1
	Canabidiol	LL167062023	1
	Canabidiol	LL181092023	3
	Canabidiol	LL186102023	2
	Canabidiol	LL198012024	1
	Canabidiol	l174122021	1
	Canabidiol	LL86022022	1
Adex Pharma	Canabidiol	100493	1
Adrex / AH	Canabidiol	100492	1
Adrex / Alli. HC	Canabidiol	100505	1
Adrex / Anzag	Canabidiol	100493	1
Adrex / Gehe	Canabidiol	100492	1
Adrex / Gehe	Canabidiol	100493	2
Adrex / Gehe	Canabidiol	100505	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Adrex / Gehe	Canabidiol	100506	1
Adrex / Gehe	Canabidiol	19Y21748	1
Adrex / Jenne	Canabidiol	100504	1
Adrex / Jenne	Canabidiol	100505	1
Adrex / Jenne	Canabidiol	19Y21746	5
Adrex / Jenne	Canabidiol	LL118092022	1
Adrex / Jenne	Canabidiol	LL35072021	2
Adrex / Jenne	Canabidiol	LL61102021	4
Adrex / Jenne	Canabidiol	LL74122021	5
Adrex / Jenne	Canabidiol	LL75122021	1
ADREX / Sana	Canabidiol	100441	1
ADREX / Sana	Canabidiol	100462	1
Adrex / Sanacorp	Canabidiol	100462	1
Adrex /Gehe 07.03.22...	Canabidiol	LL50092021	1
Adrex /Gehe 17.09.21	Canabidiol	LL31072021	1
Adrex /Phönix 14.03....	Canabidiol	LL137022023	1
Adrex gEHE	Canabidiol	100461	1
adrex Gehe	Canabidiol	100462	1
Adrex pharm	Canabidiol	100461	2
Adrex pharm	Canabidiol	100462	2
Adrex pharm	Canabidiol	100506	1
Adrex Pharm	Canabidiol	100506	1
Adrex pharm	Canabidiol	100578	1
adrex pharm	Canabidiol	13956-29-1	1
Adrex Pharma / AHD 2...	Canabidiol	100505	1
Adrex Pharma / AHD	Canabidiol	LL35072021	1
Adrex Pharma / Phoenix	Canabidiol	LL115082022	1
Adrex Pharma / Phoenix	Canabidiol	LL62102021	1
Adrex Pharma / Phoenix	Canabidiol	LL63102021	1
Adrex Pharma / Sanacorp	Canabidiol	19Y21748	2
Adrex Pharma GmbH	Canabidiol	100462	1
Adrex Pharma GmbH	Canabidiol	1133072021	1
Adrex Pharma GmbH	Canabidiol	LL33072021	1
Adrex Pharma/ Gehe	Canabidiol	LL50092021	1
Adrex Pharma/ Jenne	Canabidiol	LL74122021	3
Adrex Pharma/ Noweda	Canabidiol	100506	1
Adrex Pharma/ Noweda	Canabidiol	19Y21748	1
Adrex Pharma/ Phönix	Canabidiol	100506	1
Adrex Pharma/ Phönix	Canabidiol	LL63102021	1
Adrex Pharma/ Sanacorp	Canabidiol	100492	2
Adrex Pharma/4	Canabidiol	100442	1
Adrex Pharma/AEP	Canabidiol	100440	1
Adrex Pharma/Jenne	Canabidiol	LL62102021	1
Adrex Pharma/Noweda	Canabidiol	100442	1
Adrex Pharma/Noweda	Canabidiol	100462	1
Adrex pharma/Sanacorp	Canabidiol	LL32072021	1
adrex Pharma	Canabidiol	100442	2
ADREX pharma	Canabidiol	100460	2
Adrex Pharma	Canabidiol	100461	1
Adrex Pharma	Canabidiol	100492	2
Adrex Pharma	Canabidiol	100505	3
adrex pharma	Canabidiol	100506	1
Adrex pharma	Canabidiol	19Y21746	4
Adrex Pharma	Canabidiol	19Y21746	1
Adrex Pharma	Canabidiol	19Y21748	2
Adrex Pharma	Canabidiol	LL50092021	1
Adrex pharma	Canabidiol	LL61102021	2
Adrex Pharma	Canabidiol	LL75122021	1
ADREX/ Jenne	Canabidiol	100504	1
Adrex/AEP	Canabidiol	100493	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Adrex/AHD	Canabidiol	LL115082022	1
Adrex/AHD	Canabidiol	LL117092022	1
Adrex/AHD	Canabidiol	LL120102022	1
Adrex/AHD	Canabidiol	LL97042022	1
Adrex/Anzag	Canabidiol		1
Adrex/Anzag	Canabidiol	10(100492)	1
Adrex/Anzag	Canabidiol	100440	1
Adrex/Anzag	Canabidiol	11(100492)	1
Adrex/Anzag	Canabidiol	12(100492)	1
Adrex/Anzag	Canabidiol	13(100505)	1
Adrex/Anzag	Canabidiol	14(100492)	1
Adrex/Anzag	Canabidiol	220504(LL61102021)	1
Adrex/Gehe	Canabidiol	100461	1
Adrex/Gehe	Canabidiol	LL62102021	1
Adrex/Gehe	Canabidiol	LL75122021	5
Adrex/Gehe	Canabidiol	LL97042022	3
Adrex/Jenne	Canabidiol	211020(LL35072021)	1
Adrex/Jenne	Canabidiol	220110(19Y21746)	1
Adrex/Jenne	Canabidiol	220307(LL61102021)	1
Adrex/Jenne	Canabidiol	220428(LL61102021)	1
Adrex/Jenne	Canabidiol	220715(LL97042022)	1
Adrex/Jenne	Canabidiol	LL35072021	1
Adrex/Noweda 20.10.2021	Canabidiol	LL35072021	1
Adrex/Noweda	Canabidiol	100441	2
Adrex/Noweda	Canabidiol	100460	3
Adrex/Noweda	Canabidiol	100461	2
Adrex/Noweda	Canabidiol	100493	1
Adrex/Noweda	Canabidiol	100504	1
Adrex/Phoenix	Canabidiol	100462	1
Adrex/Phoenix	Canabidiol	LL110072022	2
Adrex/Phön 07.11.22 …	Canabidiol	LL115082022	1
Adrex/Phön 6.01.23 E…	Canabidiol	LL120102022	1
Adrex/Phönix 02.09.2…	Canabidiol	LL110072022	1
Adrex/Phönix 12.07.2…	Canabidiol	LL97042022	1
Adrex/Phönix 17.05.2…	Canabidiol	LL75122021	1
Adrex/Phönix	Canabidiol	100493	1
Adrex/Phönix	Canabidiol	100505	2
Adrex/Phönix	Canabidiol	LL35072021	2
Adrex/Phönix	Canabidiol	LL61102021	2
Adrex/Sanacorp	Canabidiol	100441	1
Adrex/Sanacorp	Canabidiol	100460	4
Adrex	Canabidiol	100442	2
Adrex	Canabidiol	100491	1
Adrex	Canabidiol	100505	1
ADREX	Canabidiol	100505	1
Adrex	Canabidiol	19Y21746	2
Adrex	Canabidiol	LL117092022	1
Adrex	Canabidiol	LL130122022	1
Adrex	Canabidiol	LL35072021	1
adrex	Canabidiol	LL48092021	1
adrex	Canabidiol	LL49092021	1
Adrex	Canabidiol	LL49092021	1
Adrex	Canabidiol	LL61102021	2
adrex	Canabidiol	LL62102021	1
Adrex	Canabidiol	LL63102021	1
Adrex	Canabidiol	LL75122021	2
Adrex	Canabidiol	LL82012022	1
adrex	Canabidiol	l184022022	1
Adrexa/Jenne	Canabidiol	19Y21746	1
Adrex-Noweda	Canabidiol	100505	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
ADREXpharma - Sanacorp	Canabidiol	100441	1
Adrexpharma / Sanacorp	Canabidiol	100461	1
ADREXpharma GmbH/Phönix	Canabidiol	19Y21746	3
ADREXpharma GmbH	Canabidiol	100400	1
ADREXpharma GmbH	Canabidiol	100442	1
ADREXpharma GmbH	Canabidiol	100462	1
ADREXpharma GmbH	Canabidiol	100491	1
ADREXpharma GmbH	Canabidiol	100493	2
ADREXpharma GmbH	Canabidiol	19Y21746	1
adrexpharma GmbH	Canabidiol	LL114082022	1
adrexpharma GmbH	Canabidiol	LL117092022	2
adrexpharma GmbH	Canabidiol	LL120102022	3
ADREXpharma GmbH	Canabidiol	LL32072021	1
adrexpharma GmbH	Canabidiol	LL62102021	1
Adrexpharma GmbH	Canabidiol	LL82012022	1
ADREXpharma, Gehe	Canabidiol	100491	1
ADREXpharma, Gehe	Canabidiol	LL48092021	1
Adrexpharma/ Phoenix	Canabidiol	LL110072022	1
Adrexpharma/ Phoenix	Canabidiol	LL115082022	2
Adrexpharma/ Phoenix	Canabidiol	LL117092022	1
Adrexpharma/ Phoenix	Canabidiol	LL48092021	2
Adrexpharma/ Phoenix	Canabidiol	LL49092021	2
Adrexpharma/ Phoenix	Canabidiol	LL62102021	4
Adrexpharma/ Phoenix	Canabidiol	LL97042022	3
ADREXpharma/ Sanacorp	Canabidiol	LL32072021	1
Adrexpharma/AHD	Canabidiol	LL97042022	6
Adrexpharma/Gehe	Canabidiol	LL97042022	2
Adrexpharma/Noweda	Canabidiol	LL114082022	3
Adrexpharma/Noweda	Canabidiol	LL115082022	1
Adrexpharma/Noweda	Canabidiol	LL118092022	1
Adrexpharma/Noweda	Canabidiol	LL14082022	1
Adrexpharma/Noweda	Canabidiol	LL50092021	1
Adrexpharma/Noweda	Canabidiol	LL62102021	3
Adrexpharma/Noweda	Canabidiol	LL63102021	1
Adrexpharma/Noweda	Canabidiol	LL7092022	1
Adrexpharma/Noweda	Canabidiol	LL75122021	2
AdrexPharma	Canabidiol	100442	7
ADREXpharma	Canabidiol	100442	5
Adrexpharma	Canabidiol	100460	1
Adrexpharma	Canabidiol	100461	1
AdrexPharma	Canabidiol	100462	1
AdrexPharma	Canabidiol	100493	1
AdrexPharma	Canabidiol	100506	10
AdrexPharma	Canabidiol	19Y21746	12
ADREXpharma	Canabidiol	19Y21746	2
AdrexPharma	Canabidiol	19Y21748	13
ADREXpharma	Canabidiol	19Y21748	2
ADREXpharma	Canabidiol	19Y217848	1
AdrexPharma	Canabidiol	LL31072021	2
AdrexPharma	Canabidiol	LL32072021	1
AdrexPharma	Canabidiol	LL33072021	1
AdrexPharma	Canabidiol	LL48092021	6
AdrexPharma	Canabidiol	LL49092021	3
AdrexPharma	Canabidiol	LL50092021	6
Adrexpharma	Canabidiol	LL62102021	1
AEP/Adrexpharma Gmbh	Canabidiol	100492	1
Alliance Healthcare	Canabidiol	100441	1
Alliance Healthcare	Canabidiol	100492	2
Alliance Healthcare	Canabidiol	19Y21748	1
Alliance Healthcare	Canabidiol	22263A	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Alliance Healthcare	Canabidiol	22398B	1
Alliance Healthcare	Canabidiol	KI0007	1
Alliance Healthcare	Canabidiol	LL32072021	1
Alliance Healthcare	Canabidiol	LL62102021	1
Alliance Healthcare	Canabidiol	LL75122021	1
alpha -Cannabis Phar...	Canabidiol	ACPL418001	1
Alpha Cannabis pharm...	Canabidiol	ACPL418001	1
alpha Cannabis/ApoCa...	Canabidiol	ACPM810901	6
Alpha Cannabis/Apoca...	Canabidiol	ACPL418001	1
alpha cannabis	Canabidiol	ACPL416001	1
alpha-cannabis 09.07.20	Canabidiol	ACPLO09001P-200709-4	1
alpha-cannabis 10.08.20	Canabidiol	ACPLO0900P-200810-1	1
alpha-cannabis 31.03.20	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol	ACPLO	1
alpha-cannabis Pharm...	Canabidiol	ACPLO09001	5
alpha-cannabis Pharm...	Canabidiol	ACPM810901	4
alpha-cannabis Pharm...	Canabidiol	ACLP416001	1
alpha-cannabis Pharm...	Canabidiol	ACPK012405	1
alpha-cannabis Pharm...	Canabidiol	ACPK911004	3
alpha-cannabis Pharm...	Canabidiol	ACPL416001	3
alpha-cannabis Pharm...	Canabidiol	ACPLO09001	2
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol	ACPL418001P190711-1	1
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol	ACPK012405P190430-2	1
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol	ACPK012405P190405-1	1
alpha-cannabis Pharm...	Canabidiol		1
alpha-cannabis Pharm...	Canabidiol	ACPL418001P-190613-2	1
alpha-cannabis Pharm...	Canabidiol	ACPK312001	1
alpha-cannabis Pharm...	Canabidiol	ACPK91100P-181220-1	1
alpha-cannabis Pharm...	Canabidiol	ACPL41800P-190527-2	1
alpha-cannabis Pharma	Canabidiol	ACPK312001	2
alpha-cannabis Pharma	Canabidiol	ACPL416001	2
alpha-cannabis Pharma	Canabidiol	ACPL418001	2
Alpha-Cannabis Pharma	Canabidiol	ACPN920903	2
Alpha-Cannabis Pharma	Canabidiol	ACPP310901	3
Andrex	Canabidiol	19y21748	1
Anzag/Adrex Pharma	Canabidiol	100441	5
Anzag/Adrex Pharma	Canabidiol	100461	8
Anzag/trigal	Canabidiol	F190205	1
ApoCare GmbH	Canabidiol	ACPLO09001	11
Apocare Pharma 11.05.20	Canabidiol		1
Apocare Pharma 15.06.2020	Canabidiol		1
Apocare Pharma 16.12.19	Canabidiol	ACPL009001P-191216-1	1
APOCARE Pharma GmbH	Canabidiol	ACPL416001	3
APOCARE Pharma GmbH	Canabidiol	ACPL418001	1
Apocare Pharma	Canabidiol		1
Apocare Pharma	Canabidiol	ACPL416001	1
Apocare	Canabidiol	ACPK312001	1
Apocare	Canabidiol	ACPK911004	9
Apocare	Canabidiol	ACPL418001	3
Apocare	Canabidiol	ACPLO09001	1
Ardex / Noweda	Canabidiol	LL75122021	3
Ardex / Noweda	Canabidiol	LL97042022	8
Ardex/Noweda	Canabidiol	19Y21746	1
Ardrex PH./Phönix	Canabidiol	100462	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Arevipharma GmbH/ Phoenix	Canabidiol		3
Arevipharma GmbH/ Phoenix	Canabidiol	100505	5
Arevipharma GmbH/ Phoenix	Canabidiol	19Y21746	1
BAFA GmbH	Canabidiol		1
Bombastus	Canabidiol		1
BSPG Lab. Ltd UK/Can...	Canabidiol	CKB20ICB4TB	1
BSPG/Pharma line	Canabidiol	F181001	10
BSPG/Trigal Pharm GmbH	Canabidiol	FB181001	10
BSPG	Canabidiol	F200205	1
Caelo	Canabidiol		14
Caelo	Canabidiol	110216-02	3
Caelo	Canabidiol	16992311	1
Caelo	Canabidiol	21000530001	1
Caelo	Canabidiol	21001526003	3
Caelo	Canabidiol	21002318002	1
Caelo	Canabidiol	21002319002	13
Caelo	Canabidiol	2100239002	1
Caelo	Canabidiol	21003190004	1
Caelo	Canabidiol	22001216003	3
Caelo	Canabidiol	ACPK911004P181203-1	1
Caelo	Canabidiol	CBD-API17-003	1
Caelo	Canabidiol	CBD-API17-006	2
Caelo	Canabidiol	CBDAPI1801	2
Caelo	Canabidiol	CBDAPI1803	1
Caelo	Canabidiol	F190205	1
Caesar & Loretz GmbH...	Canabidiol	LL97042022	1
Caesar & Loretz GmbH...	Canabidiol	21000530001	4
Caesar & Loretz GmbH	Canabidiol	21000530001	4
Caesar & Loretz GmbH	Canabidiol	21000530003	1
Caesar & Loretz GmbH	Canabidiol	21001526004	7
Caesar & Loretz GmbH	Canabidiol	21003190001	5
Caesar & Loretz GmbH	Canabidiol	22001216007	1
Cannamedical / Phönix	Canabidiol	CKB20ICB4TB	2
Cannamedical GmbH	Canabidiol	CKB20ICB35	1
Cannamedical Pharma GmbH	Canabidiol	ckb20icb35	1
Cannamedical Pharma GmbH	Canabidiol	CKB20ICB35	1
Cannamedical Pharma GmbH	Canabidiol	CKB20ICB4TB	1
Cannamedical Pharma GmbH	Canabidiol	CKB20ICCB4TB	1
Cannamedical Pharma GmbH	Canabidiol	ckb9icbanc	1
Cannamedical Pharma	Canabidiol	CKB9ICBANC	5
Cannamedical/ Cannam...	Canabidiol	CKB9ICBANB	2
Cannamedical	Canabidiol	CKB20ICB4TB	2
CannaMedical	Canabidiol	CMB21ICB08417	1
CannAMEDICAL	Canabidiol	CMB21ICB091432	1
Cantourage/AHD	Canabidiol	22021A	5
Cantourage/Gehe	Canabidiol	22020A	1
Cantourage/Phönix	Canabidiol	2021A	1
Cantourage/Phönix	Canabidiol	22012B	5
Cantourage/Phönix	Canabidiol	22020A	1
Cantourage	Canabidiol	22012B	1
CB21 Pharma,s.r.o.	Canabidiol	LL25032021	1
Direkt Apocare Pharma	Canabidiol		1
Euro OTC	Canabidiol		3
Fagron	Canabidiol	20C12-F51-381419	2
farmako GmbH	Canabidiol	LL01022020	1
Farmako GmbH	Canabidiol	LL01022020	1
farmako Gmbh	Canabidiol	LL02022020	2
Farmbios S.p.A.	Canabidiol	100461	1
Gehe, Adrex	Canabidiol	LL32072021	1
Gehe/ ADREX pharma	Canabidiol	100441	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe/Adrex 21.1.22 E...	Canabidiol	LL63102021	1
Gehe/Adrex Pharma	Canabidiol	19Y21746	2
Gehe/Adrex	Canabidiol	100440	1
Gehe/Arevipharma Gmbh	Canabidiol	100505	1
Gehe	Canabidiol	23230C	1
Gehe	Canabidiol	LL148032023	1
Gehe	Canabidiol	LL159052023	1
Gehe	Canabidiol	LL181092023	2
Gehe	Canabidiol	LL48092021	1
Gehe	Canabidiol	LL49092021	1
Hanf Zeit	Canabidiol	AL18120401	2
Ichtyolgesellschaft ...	Canabidiol	CA20190508	1
Ilios Sante 01.04.21	Canabidiol	LL020222020	2
Ilios Sante 2.2.21	Canabidiol	LL02022020	2
Jenne / Adrex	Canabidiol	100505	4
Jenne / Adrex	Canabidiol	19Y21746	2
Jenne / Adrex	Canabidiol	19Y21748	4
Jenne / Adrex	Canabidiol	LL120102022	1
Jenne / Adrex	Canabidiol	LL32072021	1
Jenne / Adrex	Canabidiol	LL50092021	1
Jenne / Trigal Pharma	Canabidiol	F190205	1
Jenne / Trigal Pharma	Canabidiol	F190703E	1
Jenne / Trigal Pharma	Canabidiol	F190704	1
Jenne	Canabidiol	ACPN920901	1
Krieger am 5.3.und7....	Canabidiol	19Y21746	3
Laborchemie APOLDA GmbH	Canabidiol	APCK312001	1
Noweda/Arex	Canabidiol	LL82012022	2
Noweda/THC Pharm	Canabidiol		6
Noweda	Canabidiol	100440	1
Noweda	Canabidiol	100505	2
Noweda	Canabidiol	16013039	1
Noweda	Canabidiol	LL164062023	1
Noweda	Canabidiol	LL181092023	1
Noweda	Canabidiol	LL62102021	1
Noweda	Canabidiol	LL72112021	1
Pharmachem GmbH & Co. KG	Canabidiol		4
Pharmachem GmbH & Co. KG	Canabidiol	CBDAPI1801	2
Phoenix / Adrexpharma	Canabidiol	LL63102021	1
Phoenix	Canabidiol	LL77122021	1
Phönix/THC	Canabidiol	1C240220-2	1
Phönix	Canabidiol		1
Phönix	Canabidiol	19Y21747	1
Sanacorp /Adrex Pharma	Canabidiol	100441	2
Sanacorp Stralsund	Canabidiol	LL63102021	1
Sanacorp/Adrex	Canabidiol	100461	1
Sanacorp	Canabidiol		6
Sanacorp	Canabidiol	CBDAPI1804	3
Sanum	Canabidiol	22020A	3
SANUM-Kehlbeck GmbH&Co.KG	Canabidiol	22397A	1
SANUM-Kehlbeck/AHD	Canabidiol	22263A	3
SANUM-Kehlbeck/AHD	Canabidiol	22398B	4
SANUM-Kehlbeck/Phönix	Canabidiol	22262B	1
Sanum-Kehlbeck	Canabidiol	22020A	1
SolMic BioTechGmbH	Canabidiol	100492	3
Spectrum Therapeutics	Canabidiol	CBD2105A02	2
Spectrum Therapeutis...	Canabidiol	CBD2105A02	1
Spectrum Therapeutis...	Canabidiol	VC2002-007	1
Spectrum	Canabidiol		1
Sterling Pharma/ Phoenix	Canabidiol	LL32072021	7
Sterling Pharma	Canabidiol	LL35072021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
THC Pharm / THC Pharm	Canabidiol		1
THC Pharm GmbH / THC…	Canabidiol	CBD-API17-005	1
THC Pharm GmbH The …	Canabidiol		4
THC Pharm GmbH/Noweda	Canabidiol	10C080421-3	4
THC Pharm GmbH/Noweda	Canabidiol	10C090421-2	1
THC Pharm GmbH/Noweda	Canabidiol	10C150121-1	3
THC Pharm GmbH/Noweda	Canabidiol	10C150321-1	2
THC Pharm GmbH/Noweda	Canabidiol	10C150321-2	2
THC Pharm GmbH/Noweda	Canabidiol	10C150321-3	3
THC Pharm GmbH/Phönix	Canabidiol		2
THC Pharm GmbH/Phönix	Canabidiol	10C080421-1	1
THC Pharm GmbH/Phönix	Canabidiol	10C150321-1	1
THC Pharm GmbH/Phönix	Canabidiol	10C160321-2	1
thc pharm gmbh	Canabidiol		3
THC Pharm GmbH	Canabidiol		94
THC Pharm GmbH	Canabidiol	100493	1
THC Pharm GmbH	Canabidiol	10C041219-0	1
THC Pharm GmbH	Canabidiol	10C121119-2	1
THC Pharm GmbH	Canabidiol	10C180520	1
THC Pharm GmbH	Canabidiol	10C180520-0	3
THC Pharm GmbH	Canabidiol	1C031219-0	5
THC Pharm GmbH	Canabidiol	CBD-API17-005	3
THC Pharm GmbH	Canabidiol	CBD-API17-006	2
THC Pharm GmbH	Canabidiol	CBDAPI1707	2
THC Pharm GmbH	Canabidiol	CBDAPI1801	3
THC Pharm GmbH	Canabidiol	CBDAPI1802	1
THC Pharm GmbH	Canabidiol	CBDAPI1804	2
THC Pharm GmbH	Canabidiol	CBDAPI1805	5
THC Pharm GmbH	Canabidiol	S20-017	1
THC Pharm/ direkt	Canabidiol		8
THC Pharm/ Noweda	Canabidiol		2
THC Pharm/ THC Pharm GmbH	Canabidiol		1
THC Pharm/ THC Pharm	Canabidiol		2
THC Pharm/AHD	Canabidiol		1
THC PHARM/GEHE	Canabidiol		2
THC Pharm/Phönix	Canabidiol		2
THC Pharm/THC Pharma	Canabidiol		1
Thc Pharm	Canabidiol		1
THC Pharm	Canabidiol		126
THC PHARM	Canabidiol		1
THC Pharm	Canabidiol	10C140819-1	1
THC Pharm	Canabidiol	10C170619-1	1
THC Pharm	Canabidiol	CA20190507_01	1
THC Pharm	Canabidiol	CA20190508_01	1
THC Pharm	Canabidiol	CA20190508_02	1
THC PHARM	Canabidiol	CBD2006A01	1
THC PHARM	Canabidiol	CBD2007A03	1
THC PHARM	Canabidiol	CBD2107A02	1
THC Pharm	Canabidiol	CBD-API16-004	6
THC Pharm	Canabidiol	CBD-API17-004	1
THC Pharm	Canabidiol	CBD-API17-006	2
THC Pharm	Canabidiol	CBDAPI1707	1
THC Pharm	Canabidiol	CBDAPI1708	2
THC Pharm	Canabidiol	CBDAPI1802	2
THC Pharm	Canabidiol	CBDAPI1804	5
THC Pharm	Canabidiol	CBDAPI1901	1
THC Pharm	Canabidiol	CBDAPL1802	1
THC Pharm	Canabidiol	H150218-1	1
THC Pharma (direkt)	Canabidiol		2
THC Pharma (direkt)	Canabidiol	CBD-API17-006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
THC Pharma (direkt)	Canabidiol	CBDAPI1707	1
THC Pharma (direkt)	Canabidiol	CBDAPI1708	1
THC Pharma (direkt)	Canabidiol	CBDAPI1801	1
THC Pharma / Cansati...	Canabidiol		5
THC PHARMA GMBH	Canabidiol	1C010420-2	1
THC Pharma/ Phönix	Canabidiol		23
THC Pharma/ Phönix	Canabidiol	10C060421-0	3
THC Pharma/ THC Pharma	Canabidiol		1
Thc Pharma/Gehe	Canabidiol		6
THC Pharma/Gehe	Canabidiol		1
THC Pharma/Noweda	Canabidiol		1
THC Pharma/Noweda	Canabidiol	10C250220-1	1
THC Pharma/Phönix	Canabidiol		36
THC Pharma/Phönix	Canabidiol	10C010420-2	4
THC Pharma/Phönix	Canabidiol	10C180520-0	1
THC Pharma/Phönix	Canabidiol	10C300320-3	4
THC Pharma/THC Pharma	Canabidiol		2
THC pharma	Canabidiol		3
THC Pharma	Canabidiol		234
THC Pharma	Canabidiol	10C180520-0	2
THC Pharma	Canabidiol	1C210619-1	6
THC Pharma	Canabidiol	CBD2108A02	1
THC Pharma	Canabidiol	CBDAP/1801	1
THC Pharma	Canabidiol	CBD-API16-004	3
THC Pharma	Canabidiol	CBD-API17-002	5
THC Pharma	Canabidiol	CBD-API17-004	9
THC Pharma	Canabidiol	CBD-API17-005	6
THC Pharma	Canabidiol	CBDAPI1706	4
THC Pharma	Canabidiol	CBDAPI1707	2
THC Pharma	Canabidiol	CBDAPI1802	4
THC Pharma	Canabidiol	CBDAPI1803	1
THC Pharma	Canabidiol	CBDAPI1804	6
THC Pharma	Canabidiol	CBDAPI1901	3
THC Pharma	Canabidiol	CBDAPI2003	1
THC Pharma	Canabidiol	CBDAPI2008	1
THC PHRMA	Canabidiol		18
THC PHRMA	Canabidiol	1C090519-1	1
THC Spectrum	Canabidiol		4
THC/ Direkt	Canabidiol	CBDAPI1706	1
THC/ THC	Canabidiol		2
THC/Gehe	Canabidiol	CBD-API17-005	1
THC/THC	Canabidiol		2
THC	Canabidiol		47
THC	Canabidiol	10C150321-1	1
THC	Canabidiol	14295559	1
THC	Canabidiol	CBD-API17-002	2
THC	Canabidiol	CBD-API17-003	1
THC	Canabidiol	CBD-API17-004	4
THC	Canabidiol	CBD-API17-006	2
Thcph	Canabidiol		1
THC-Pharm/Phoenix	Canabidiol		1
THC-Pharm	Canabidiol		13
THC-Pharm	Canabidiol	cbd-adi17-002	1
THC-Pharm	Canabidiol	CBDAP/17-003	3
THC-Pharm	Canabidiol	CBD-API17-004	1
THC-Pharm	Canabidiol	CBD-API17-005	1
THC-Pharma GmbH	Canabidiol		7
THC-Pharma	Canabidiol		21
THC-PHARMA	Canabidiol	1C140819-0	5
THC-Pharma	Canabidiol	CBDAP/1708	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
THC-Pharma	Canabidiol	CBD-API17-003	1
THC-Pharma	Canabidiol	CBDAPI1708	1
THC-Pharma	Canabidiol	CBDAPI1802	1
THC-Pharma	Canabidiol	CBDAPI1804	1
THC-Pharma	Canabidiol	CBDAPI1904	1
TRIGAL Pharma GmbH	Canabidiol	F200205	1
Trigal Pharma	Canabidiol	F200205	1
Trigal/Gehe	Canabidiol	F190205K	11
Trigal/Gehe	Canabidiol	F200205	10
Trigal/Gehe	Canabidiol	F200208	6
Trigal/Gehe	Canabidiol	F200701	31
Trigal/Phoenix	Canabidiol	F190205	11
Trigal/Phoenix	Canabidiol	F190704	8

- 234 360 spectra from 1515 *Apo-Ident* customers from a total of 48 969 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Canabidiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Canabidiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	760	0	152 202
Type B	0	871	0	201 213
Type C	0	1705	2	234 360

The substance/substance group *Canabidiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2105 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3111 %)
Type C	100.0000 % (> 99.9007 %)	99.8828 % (> 99.7071 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22412	22412	0,00	99,83
22413	22413	0,00	100,15
22414	22414	0,00	100,26
22415	22415	0,00	100,22
22416	22416	0,00	99,66
23398	22413	6,37	100,21
23399	23465	7,46	100,71
23464	23464	0,00	101,82
23465	23465	0,00	98,95
25504	22415	8,06	100,74
25612	25612	0,00	102,68
25995	25995	0,00	102,55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cânfora racêmica/cânfora D**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	25048-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cânfora racêmica/cânfora D; Camphora racemica; Cânfora D; Cânfora racêmica; D-Camphora

Special notes

When selecting the *Cânfora racêmica/cânfora D* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cânfora racêmica/cânfora D	10	11	81

Second-stage model

For differentiation of the substance/substance group *Cânfora racêmica/cânfora D* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cânfora racêmica/cânfora D* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Espironolactona	76,52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cânfora racêmica/cânfora D* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cânfora racêmica/cânfora D*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cânfora D	162354	24680	40	20160809*
Caelo	Cânfora D	23000933	27262	40	20230505*
Gatt-Koller	Cânfora D	23J02066	27091	40	20231109
Gatt-Koller	Cânfora D	23J02066	27091SI	20	20231109
Caelo	Cânfora racêmica	15316801	25049	60	20151029
Caelo	Cânfora racêmica	170043	25051	40	20170220*
Caelo	Cânfora racêmica	192762	25562	40	20200127*
Caelo	Cânfora racêmica	21002072014	25977	40	20210817
Euro OTC	Cânfora racêmica	1406029-01	25048	60	20140708
Fagron	Cânfora racêmica	14E19-B07-300365	25050	60	20140527
Fagron	Cânfora racêmica	16E23-B08-336937	25053	40	20160627

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Cânfora racêmica/cânfora D*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 482 spectra from a total of 2832 batches from further 484 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 500 spectra of 15 reference samples from the substance/substance group *Cânfora racêmica/cânfora D*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cânfora D	190097	24681	40
Caelo	Cânfora racêmica	183279	24728	40
Caelo	Cânfora racêmica	192454	24876	40
Caelo	Cânfora racêmica	16209309	25052	40
Caelo	Cânfora racêmica	172883	25054	40
Caelo	Cânfora racêmica	180198	25055	40
Caelo	Cânfora racêmica	21003662	25994	40
Caelo	Cânfora racêmica	23001930	26947	40
Caelo	Cânfora racêmica	24001181	27259	40
Fagron	Cânfora racêmica	21K27-B05-226181	26462	40
Gatt-Koller	Cânfora racêmica	21J02080	26704	40
Caelo	Cânfora D	23000933	27262SI†	20
Caelo	Cânfora racêmica	21002072014	25977SI†	10
Caelo	Cânfora racêmica	21003662	25994SI	10
Fagron	Cânfora racêmica	21K27-B05-226181	26462SI	20

- 201 584 spectra from a total of 4032 batches from further 841 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 362 spectra from 240 *Apo-Ident* customers from 82 batches from the substance/substance group *Cânfora racêmica/cânfora D.*
- Among them are spectra of independent samples from 81 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cânfora racêmica	16235408	1
	Cânfora racêmica	21000070022	1
	Cânfora racêmica	21003662006	2
	Cânfora racêmica	21003662010	6
	Cânfora racêmica	21003662011	1
	Cânfora racêmica	22003278003	1
	Cânfora racêmica	22003278004	3
	Cânfora racêmica	22003278007	3
	Cânfora racêmica	2203278007	1
	Cânfora racêmica	24000108001	1
AHD	Cânfora racêmica	192762005	1
Alliance Healthcare	Cânfora racêmica	18196907	2
Alliance Healthcare	Cânfora racêmica	22001161003	1
Caelo	Cânfora racêmica	17004301	1
Caelo	Cânfora racêmica	17050605	2
Caelo	Cânfora racêmica	17288306	2
Caelo	Cânfora racêmica	17288307	2
Caelo	Cânfora racêmica	18019806	5
Caelo	Cânfora racêmica	18066404	1
Caelo	Cânfora racêmica	18108904	1
Caelo	Cânfora racêmica	18196906	5
Caelo	Cânfora racêmica	18196907	8
Caelo	Cânfora racêmica	183279001	1
Caelo	Cânfora racêmica	183279002	10
Caelo	Cânfora racêmica	18327901	1
Caelo	Cânfora racêmica	18327903	5
Caelo	Cânfora racêmica	18327905	12
Caelo	Cânfora racêmica	18327909	20
Caelo	Cânfora racêmica	18327910	1
Caelo	Cânfora racêmica	19009704	4
Caelo	Cânfora racêmica	19245003	1
Caelo	Cânfora racêmica	192454002	1
Caelo	Cânfora racêmica	192454003	1
Caelo	Cânfora racêmica	192454004	6
Caelo	Cânfora racêmica	192454006	8
Caelo	Cânfora racêmica	19262009	1
Caelo	Cânfora racêmica	192762002	1
Caelo	Cânfora racêmica	192762004	3
Caelo	Cânfora racêmica	192762005	8
Caelo	Cânfora racêmica	192762007	2
Caelo	Cânfora racêmica	192762009	16
Caelo	Cânfora racêmica	192823001	1
Caelo	Cânfora racêmica	192823004	1
Caelo	Cânfora racêmica	200003828001	1
Caelo	Cânfora racêmica	20003828001	10
Caelo	Cânfora racêmica	20003828002	3
Caelo	Cânfora racêmica	20003828003	1
Caelo	Cânfora racêmica	20003828006	3
Caelo	Cânfora racêmica	20004261006	6
Caelo	Cânfora racêmica	20004261007	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cânfora racêmica	21000070001	1
Caelo	Cânfora racêmica	21000070003	1
Caelo	Cânfora racêmica	21000070008	1
Caelo	Cânfora racêmica	21000070011	1
Caelo	Cânfora racêmica	21000070022	1
Caelo	Cânfora racêmica	210020720009	1
Caelo	Cânfora racêmica	21002072001	5
Caelo	Cânfora racêmica	21002072002	8
Caelo	Cânfora racêmica	21002072009	5
Caelo	Cânfora racêmica	21002072013	1
Caelo	Cânfora racêmica	21002072014	5
Caelo	Cânfora racêmica	210020722002	1
Caelo	Cânfora racêmica	21003662002	7
Caelo	Cânfora racêmica	21003662003	1
Caelo	Cânfora racêmica	21003662006	6
Caelo	Cânfora racêmica	21003662010	2
Caelo	Cânfora racêmica	2102072002	1
Caelo	Cânfora racêmica	22003278007	1
Caelo	Cânfora racêmica	5218Q-01221	1
Caelo	Cânfora racêmica	63(192454004)	1
Caelo	Cânfora racêmica	Caelo	1
Caelo	Cânfora racêmica	Nachreichen	1
Caesar & Lorenz GmbH	Cânfora racêmica	192762005	1
Caesar & Loretz GmbH…	Cânfora racêmica	21002072002	1
Caesar & Loretz GmbH…	Cânfora racêmica	18327901	1
Caesar & Loretz GmbH…	Cânfora racêmica	21002072002	1
Caesar & Loretz GmbH…	Cânfora racêmica	21002072014	1
Caesar & Loretz GmbH…	Cânfora racêmica	21003662010	1
Caesar & Loretz GmbH/AHD	Cânfora racêmica	21002072014	1
Caesar & Loretz GmbH…	Cânfora racêmica	20003828001	1
Caesar & Loretz GmbH/Gehe	Cânfora racêmica	183279	1
Caesar & Loretz GmbH/Now	Cânfora racêmica	20003828001	1
Caesar & Loretz GmbH…	Cânfora racêmica	183279002	1
Caesar & Loretz GmbH…	Cânfora racêmica	18327905	1
Caesar & Loretz GmbH/Otto	Cânfora racêmica	192762005	1
Caesar & Loretz GmbH…	Cânfora racêmica	20004261007	1
Caesar & Loretz GmbH…	Cânfora racêmica	192762007	1
Caesar & Loretz GmbH/Sa	Cânfora racêmica	18327901	1
Caesar & Loretz GmbH…	Cânfora racêmica	18327909	1
Caesar & Loretz GmbH…	Cânfora racêmica	21003662010	1
Caesar & Loretz GmbH	Cânfora racêmica	17288306	3
Caesar & Loretz GmbH	Cânfora racêmica	18019807	1
Caesar & Loretz GmbH	Cânfora racêmica	18019811	1
Caesar & Loretz GmbH	Cânfora racêmica	18196906	2
Caesar & Loretz GmbH	Cânfora racêmica	18196907	1
Caesar & Loretz GmbH	Cânfora racêmica	183279002	2
Caesar & Loretz GmbH	Cânfora racêmica	18327903	2
Caesar & Loretz GmbH	Cânfora racêmica	18327905	3
Caesar & Loretz GmbH	Cânfora racêmica	18327909	5
Caesar & Loretz GmbH	Cânfora racêmica	18327910	4
Caesar & Loretz GmbH	Cânfora racêmica	192454001	1
Caesar & Loretz GmbH	Cânfora racêmica	192454004	7
Caesar & Loretz GmbH	Cânfora racêmica	192454006	3
Caesar & Loretz GmbH	Cânfora racêmica	192454007	1
Caesar & Loretz GmbH	Cânfora racêmica	192762001	1
Caesar & Loretz GmbH	Cânfora racêmica	192762005	2
Caesar & Loretz GmbH	Cânfora racêmica	192762009	8
Caesar & Loretz GmbH	Cânfora racêmica	20003828001	8
Caesar & Loretz GmbH	Cânfora racêmica	20003828002	2
Caesar & Loretz GmbH	Cânfora racêmica	20003828006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cânfora racêmica	20004261002	1
Caesar & Loretz GmbH	Cânfora racêmica	20004261005	1
Caesar & Loretz GmbH	Cânfora racêmica	20004261006	1
Caesar & Loretz GmbH	Cânfora racêmica	20004261007	2
Caesar & Loretz GmbH	Cânfora racêmica	21002072001	2
Caesar & Loretz GmbH	Cânfora racêmica	21002072002	3
Caesar & Loretz GmbH	Cânfora racêmica	21002072009	4
Caesar & Loretz GmbH	Cânfora racêmica	21002072012	1
Caesar & Loretz GmbH	Cânfora racêmica	21002072013	1
Caesar & Loretz GmbH	Cânfora racêmica	21002072014	3
Caesar & Loretz GmbH	Cânfora racêmica	21003662002	3
Caesar & Loretz GmbH	Cânfora racêmica	21003662003	1
Caesar & Loretz GmbH	Cânfora racêmica	21003662006	3
Caesar&Loretz GmbH	Cânfora racêmica	192454004	1
Caleo/Phoenix	Cânfora racêmica	21002072009	1
campher racemischer	Cânfora racêmica	21003662010	1
EuRho/Phönix	Cânfora racêmica	21002072002	1
Euro OTC	Cânfora racêmica	1202021	1
FIEBIG	Cânfora racêmica	110-01	1
Gehe	Cânfora racêmica	21003662010	1
Kehr	Cânfora racêmica	21003662006	2
Klenk	Cânfora racêmica	444A180815	5
Klenk	Cânfora racêmica	444A200110-01	1
Noveda	Cânfora racêmica	192762009	1
Noweda	Cânfora racêmica	21002072014	1
Noweda	Cânfora racêmica	22001161005	1
Oriental/Noweda	Cânfora racêmica	102/1819	1
Orientel Aromatics	Cânfora racêmica	192762009	1
Phoenix	Cânfora racêmica	192762002	1
Phönix	Cânfora racêmica	183279002	1
Phönix	Cânfora racêmica	21002072002	1
Sanacorp	Cânfora racêmica	18327903	1
Sanacorp	Cânfora racêmica	21000070026	1

- 235 705 spectra from 1515 *Apo-Ident* customers from a total of 49 200 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cânfora racêmica/cânfora D* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cânfora racêmica/cânfora D* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	500	0	201 584
Type C	0	361	1	234 979

The substance/substance group *Cânfora racêmica/cânfora D* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.9005 %)	99.7238 % (> 98.8950 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24680	24680	0,00	170,44
25048	24680	11,27	171,04
25049	25562	11,13	170,60
25050	27262	9,14	170,05
25051	25051	0,00	168,33
25053	24680	10,05	169,71
25562	25562	0,00	168,93
25977	24680	35,84	162,72
27091	25562	19,44	169,59
27262	27262	0,00	167,46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Capsaicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20854-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Capsaicina; Capsacinum

Special notes

When selecting the *Capsaicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Capsaicina	6	5	14

Second-stage model

For differentiation of the substance/substance group *Capsaicina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Capsaicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	55,17	–
⋮	⋮	⋮
Alfaestradiol	>50	55,29
Citrato de sódio	>50	114,99
Levocarnitina	>50	231,46
Prednicarbato	>50	257,71
Cloridrato de oxibutinina	>50	264,49
Tetracaína	>50	276,62
Acetato de noretisterona	>50	369,35
Heparina sódica	>50	373,66
Cloridrato de quinina di-hidratado	>50	386,48
Acetato de ciproterona	>50	454,03
Piridoxal-5-fosfato	>50	493,33
Metoxisaleno	>50	730,08
Cloridrato de ciprofloxacina	>50	846,81
Amifampridina	>50	897,27
Cloridrato de amitriptilina	>50	999,16
Sacarose	>50	1242,77
Triclosan	>50	1381,59
Valina	>50	1550,48

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Capsaicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Capsaicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Capsaicina	118066-04	21638	60	20140227
Euro OTC	Capsaicina	1703023	23145	40	20170407*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Capsaicina	1811009	24331	40	20181207*
Euro OTC	Capsaicina	2003046	25258	40	20200701*
Fagron	Capsaicina	13D12-N01	20854	40	1411392
Fagron	Capsaicina	13J07-N07	21340	40	AR-15-FG-007151-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Capsaicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 260 spectra of 7 reference samples from the substance/substance group *Capsaicina*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Capsaicina	1603005-01	22930	40
Euro OTC	Capsaicina	1806013-01	24186	40
Euro OTC	Capsaicina	1812015	24457	40
Euro OTC	Capsaicina	1903032	24638	40
Euro OTC	Capsaicina	2312006	27296	40
Euro OTC	Capsaicina	1603005-01	22931	40
Euro OTC	Capsaicina	2312006	27296SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 824 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 47 spectra from 31 *Apo-Ident* customers from 14 batches from the substance/substance group *Capsaicina*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Capsaicina	2003046-03	2
Caelo	Capsaicina	1603005-01	1
Caelo	Capsaicina	180601301	1
EuRho/Alliance Healthcare	Capsaicina	2003046-02	1
EuRho	Capsaicina	1703023-02	1
Euro OTC	Capsaicina	1401043-02	2
Euro OTC	Capsaicina	1603005-01	14
Euro OTC	Capsaicina	1703023-02	1
Euro OTC	Capsaicina	1703023-025346	1
Euro OTC	Capsaicina	1806013-01	2
Euro OTC	Capsaicina	1812015-01	2
Euro OTC	Capsaicina	1903032-02	5
Euro OTC	Capsaicina	19H029	1
Euro OTC	Capsaicina	2003046-02	5
Euro OTC	Capsaicina	I1812015-01	1
Euro OTC	Capsaicina	II1812015-01	1
Extraktion	Capsaicina	2003046-02	1
Fagron	Capsaicina	CP-12003	1
Gehe	Capsaicina	2003046-02	3
Noweda	Capsaicina	2003046-02	1

- 236 020 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Capsaicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Capsaicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	260	0	201 824
Type C	0	46	1	236 020

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Capsaicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.9007 %)	97.8723 % (> 91.4894 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20854	20854	0,00	109,54
21340	21340	0,00	121,89
21638	21340	14,09	137,25
23145	23145	0,00	109,90
24331	24331	0,00	133,89
25258	25258	0,00	105,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Captopril**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20890-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Captopril; Captoprilum

Special notes

When selecting the *Captopril* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Captopril	6	7	182

Second-stage model

For differentiation of the substance/substance group *Captopril* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Captopril* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	69,86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Captopril* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Captopril*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Captopril	12339610	21064	40	1403227
Caelo	Captopril	15189502	21874	60	AR-15-FG-014855-01
Caelo	Captopril	190118	24546	40	20190312*
Fagron	Captopril	12G25-N08	20890	40	20120814
Fagron	Captopril	14B26-B01-312221	21921	60	20140317
Fagron	Captopril	19I24-F01-369346	25370	40	20191031
Fagron	Captopril	19I24-F01-369346	25370SI	40	20191031

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Captopril*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 15 reference samples from the substance/substance group *Captopril*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Captopril	170772	23366	40
Caelo	Captopril	172102	23676	40
Caelo	Captopril	21001156009	25932	40
Caelo	Captopril	23002616	27225	40
Caelo	Captopril	22004035	27229	30
Fagron	Captopril	17G21-B02-337989	23588	30
Fagron	Captopril	22C03-B01-220899	26380	40
Caelo	Captopril	15189502	21874SI†	60
Caelo	Captopril	170772	23366SI	40
Caelo	Captopril	190118	24546SI†	40
Caelo	Captopril	21001156009	25932SI	40
Caelo	Captopril	23002616	27225SI	40
Caelo	Captopril	22004035	27229SI	40
Fagron	Captopril	14B26-B01-312221	21921SI†	60
Fagron	Captopril	22C03-B01-220899	26380SI	40

- 201 464 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 673 spectra from 241 *Apo-Ident* customers from 190 batches from the substance/substance group *Captopril*.

- Among them are spectra of independent samples from 181 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Captopril		1
	Captopril	21001156002	1
	Captopril	21003880005	1
	Captopril	21003880009	1
	Captopril	2100388001	1
	Captopril	21003880010	1
	Captopril	22004035001	1
	Captopril	22004035002	12
	Captopril	22004035006	3
	Captopril	22C03-B01	1
	Captopril	22C03-B01-220899	1
	Captopril	22C03-B01-230379	1
	Captopril	23002616002	1
	Captopril	EC220112	1
AHC	Captopril	23002616001	1
AHD	Captopril	22004035001	1
AHD	Captopril	22004035003	1
AHD	Captopril	23002616002	1
Bombastus	Captopril	17210202	1
Caelo	Captopril	12339602	1
Caelo	Captopril	12339604	2
Caelo	Captopril	12339605	4
Caelo	Captopril	12339610	2
Caelo	Captopril	12339616	2
Caelo	Captopril	12339617	1
Caelo	Captopril	12339619	1
Caelo	Captopril	12F29-N04	1
Caelo	Captopril	14196901	1
Caelo	Captopril	14196903	2
Caelo	Captopril	14196904	8
Caelo	Captopril	14196905	3
Caelo	Captopril	14B26-B01-291555	1
Caelo	Captopril	14B26-B01-291557	1
Caelo	Captopril	14B26-B01-310127	2
Caelo	Captopril	14B26-B40	1
Caelo	Captopril	14B26-B40-318894	1
Caelo	Captopril	14B26-B40-320183	1
Caelo	Captopril	14B26-B40-323267	2
Caelo	Captopril	14B26-B40-325275	2
Caelo	Captopril	14B26-B01-310127	1
Caelo	Captopril	15189501	6
Caelo	Captopril	15189502	1
Caelo	Captopril	15189503	1
Caelo	Captopril	15189504	1
Caelo	Captopril	15189507	3
Caelo	Captopril	15189509	3
Caelo	Captopril	15189510	2
Caelo	Captopril	15189511	5
Caelo	Captopril	15189512	11
Caelo	Captopril	15189514	6
Caelo	Captopril	15189514I-041016	1
Caelo	Captopril	15189514I-041016-2	1
Caelo	Captopril	15189515	3
Caelo	Captopril	15189517	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Captopril	15189519	2
Caelo	Captopril	15189521	5
Caelo	Captopril	15189524	2
Caelo	Captopril	15189525	2
Caelo	Captopril	15189526	2
Caelo	Captopril	1519521	1
Caelo	Captopril	16B26-B01310127	1
Caelo	Captopril	17077201	5
Caelo	Captopril	17077202	4
Caelo	Captopril	17077203	1
Caelo	Captopril	17077205	1
Caelo	Captopril	17077206	1
Caelo	Captopril	17077208	8
Caelo	Captopril	17077209	18
Caelo	Captopril	1718A-03358	1
Caelo	Captopril	17210201	6
Caelo	Captopril	17210202	16
Caelo	Captopril	17210203	1
Caelo	Captopril	17210204	5
Caelo	Captopril	17210205	10
Caelo	Captopril	17G27-B02	3
Caelo	Captopril	17G27-B02-340798	1
Caelo	Captopril	17G27-B02-342412	1
Caelo	Captopril	17G27-B02-354613	1
Caelo	Captopril	1805005	1
Caelo	Captopril	18058001	1
Caelo	Captopril	18058002	8
Caelo	Captopril	18058003	1
Caelo	Captopril	18058004	6
Caelo	Captopril	18058005	10
Caelo	Captopril	18058006	3
Caelo	Captopril	18058007	2
Caelo	Captopril	18058009	1
Caelo	Captopril	18058010	2
Caelo	Captopril	19000652002	5
Caelo	Captopril	190006520020	1
Caelo	Captopril	19000652004	9
Caelo	Captopril	19000652005	23
Caelo	Captopril	190115001	1
Caelo	Captopril	190118001	8
Caelo	Captopril	19011801	7
Caelo	Captopril	19011802	4
Caelo	Captopril	19011803	2
Caelo	Captopril	19011805	2
Caelo	Captopril	19011806	4
Caelo	Captopril	19011807	10
Caelo	Captopril	21000272002	3
Caelo	Captopril	21001156001	3
Caelo	Captopril	21001156002	14
Caelo	Captopril	21001156003	1
Caelo	Captopril	21001156005	2
Caelo	Captopril	21001156006	1
Caelo	Captopril	21001156007	5
Caelo	Captopril	21001156009	9
Caelo	Captopril	21001156010	3
Caelo	Captopril	21003880001	8
Caelo	Captopril	21003880002	2
Caelo	Captopril	21003880005	2
Caelo	Captopril	21003880006	10
Caelo	Captopril	21003880007	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Captopril	21003880009	3
Caelo	Captopril	21003880010	1
Caelo	Captopril	21003880011	2
Caelo	Captopril	2100388006	1
Caelo	Captopril	2100388009	1
Caelo	Captopril	22004035001	1
Caelo	Captopril	5102-14-042	1
Caelo	Captopril	901180021	1
Caeol/ Noweda	Captopril	15189519	1
Caeol/ Noweda	Captopril	17077202	1
Caesar & Loretz GmbH...	Captopril	19000652002	1
Caesar & Loretz GmbH...	Captopril	19011802	1
Caesar & Loretz GmbH...	Captopril	19000652005	2
Caesar & Loretz GmbH...	Captopril	21000272002	2
Caesar & Loretz GmbH/Gehe	Captopril	19011805	1
Caesar & Loretz GmbH/Gehe	Captopril	21001156003	1
Caesar & Loretz GmbH...	Captopril	19000652002	1
Caesar & Loretz GmbH...	Captopril	190118002	1
Caesar & Loretz GmbH/Kehr	Captopril	21003880007	1
Caesar & Loretz GmbH/L10	Captopril	21003880002	3
Caesar & Loretz GmbH...	Captopril	21001156002	1
Caesar & Loretz GmbH...	Captopril	19000652002	1
Caesar & Loretz GmbH...	Captopril	21001156006	1
Caesar & Loretz GmbH	Captopril	18058002	1
Caesar & Loretz GmbH	Captopril	18058006	1
Caesar & Loretz GmbH	Captopril	19000652005	3
Caesar & Loretz GmbH	Captopril	19011801	1
Caesar & Loretz GmbH	Captopril	19011802	1
Caesar & Loretz GmbH	Captopril	19011805	2
Caesar & Loretz GmbH	Captopril	19011807	1
Caesar & Loretz GmbH	Captopril	21000272002	1
Caesar & Loretz GmbH	Captopril	21001156002	2
Caesar & Loretz GmbH	Captopril	21001156003	4
Caesar & Loretz GmbH	Captopril	21001156005	1
Caesar & Loretz GmbH	Captopril	21001156007	3
Caesar & Loretz GmbH	Captopril	21001156009	3
Caesar & Loretz GmbH	Captopril	21001156010	2
Caesar & Loretz GmbH	Captopril	21003880001	2
Caesar & Loretz GmbH	Captopril	21003880005	2
Caesar & Loretz GmbH	Captopril	21003880006	2
Caesar & Loretz GmbH	Captopril	21003880007	1
Caesar & Loretz	Captopril	21001156002	1
Caesar&Loretz	Captopril	17210201	1
Cealo/Sanacorp	Captopril	12339617	1
Changzhou Pharmaceutical	Captopril	14B26-B40-321319	1
Euro OTC	Captopril	14B26-B40-320183	1
Euro OTC	Captopril	17210204	1
Euro OTC	Captopril	18058003	1
Euroct/Gehe	Captopril	14B26-B40-320183	1
Fagron	Captopril		1
Fagron	Captopril	12G25-N08	4
Fagron	Captopril	12K16-N04	1
Fagron	Captopril	12K-16N04	1
Fagron	Captopril	1369240	1
Fagron	Captopril	14196902	1
Fagron	Captopril	14B26B01	1
Fagron	Captopril	14B26-B01	6
Fagron	Captopril	14B26-B01_2911557	1
Fagron	Captopril	14B26-B01_302338	1
Fagron	Captopril	14B26-B01-291555	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Captopril	14B26-B01-291556	3
Fagron	Captopril	14B26-B01-291557	5
Fagron	Captopril	14B26-B01-302337	1
Fagron	Captopril	14B26-B01-302338	4
Fagron	Captopril	14B26-B01-310127	6
Fagron	Captopril	14B26-B01-312221	1
Fagron	Captopril	14B26-B01-314460	1
Fagron	Captopril	14B26-B01-316257	2
Fagron	Captopril	14B26-B40-318894	5
Fagron	Captopril	14B26-B40-320183	6
Fagron	Captopril	14B26-B40-321319	5
Fagron	Captopril	14B26B40323267	1
Fagron	Captopril	14B26-B40-323267	3
Fagron	Captopril	14B26-B40-325275	3
Fagron	Captopril	14B26-W0129-1557	1
Fagron	Captopril	17g27-b02-337989	1
Fagron	Captopril	17G27-B02-337989	5
Fagron	Captopril	17G27-B02-340789	1
Fagron	Captopril	17G27-B02-340798	2
Fagron	Captopril	17G27-B02-346203	2
Fagron	Captopril	17G27-B02-350227	1
Fagron	Captopril	17G27-B02-350997	1
Fagron	Captopril	17G27-B02-352730	2
Fagron	Captopril	17G27-B02-356147	6
Fagron	Captopril	17G-B02-352730	1
Fagron	Captopril	19/24-F01	1
Fagron	Captopril	19/24-F01-365391	1
Fagron	Captopril	19/24-F01-367084	1
Fagron	Captopril	19/24-F01-369346	1
Fagron	Captopril	19/24-FO1-367389	1
Fagron	Captopril	19124-F01-3692400	1
Fagron	Captopril	1924-f01-365391	1
Fagron	Captopril	1924-F01-367389	1
Fagron	Captopril	1924F01365391	1
Fagron	Captopril	19I24-F01-365390	2
Fagron	Captopril	19I24-F01-365391	5
Fagron	Captopril	19I24-F01-367084	1
Fagron	Captopril	19I24-F01-367389	1
Fagron	Captopril	19I24-F01-369240	3
Fagron	Captopril	19I24-F01-369345	1
Fagron	Captopril	19I24-F01-369346	3
Fagron	Captopril	19I24-FO1-365391	1
Fagron	Captopril	19l24-F01365391	1
Fagron	Captopril	21/15-B05-2136403	1
Fagron	Captopril	21/15-B05-213643	6
Fagron	Captopril	2115_b05_213643	1
Fagron	Captopril	21I15-B05-213643	4
Fagron	Captopril	21l15-BO5-213643	1
Fagron	Captopril	22003-B01-220899	1
Fagron	Captopril	22C03-B01	2
Fagron	Captopril	22C03-B01-220899	1
Fagron	Captopril	700766	1
Fagron	Captopril	80616-6	1
Fagron	Captopril	EC140101	1
Fagron	Captopril	EC170110	4
Fagron	Captopril	EC18019	1
Fagron	Captopril	EC181019	1
Fagron	Captopril	F01-3653901	1
Fagron	Captopril	F01-3673809	2
Fagron	Captopril	F01-3692400	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Captopril	F01-3693406	1
Fagrron	Captopril	14B26-B01-310127	2
GEHE	Captopril	17077209	1
GEHE	Captopril	17210203	1
Gehe	Captopril	18058002	1
GEHE	Captopril	18058003	1
Gehe	Captopril	18058004	2
Gehe	Captopril	18058010	1
Gehe	Captopril	19011805	2
Gehe	Captopril	21003880009	1
Gehe	Captopril	22C03-B01-234634	1
gepepharm GmbH	Captopril	21003880007	1
Hedinger	Captopril	14B26-B40	2
Herstellung	Captopril	12339607	1
Kehr	Captopril	21003880010	1
Kehr	Captopril	22004035002	3
Klosterring	Captopril	17G27-B02-340471	1
L12	Captopril	17077202	2
Noweda	Captopril	17210202	1
Noweda	Captopril	19011806	1
Noweda	Captopril	21001156009	1
Noweda	Captopril	210388010	1
Noweda	Captopril	22004035001	1
Noweda	Captopril	22004035003	1
Noweda	Captopril	220040358001	1
Noweda	Captopril	22C03-B01-230279	1
Phoenix	Captopril	22004035002	1
Phonix	Captopril	14B26-B01	1
Phönix	Captopril	18058002	1
PHÖNIX	Captopril	19124-f01-367389	1
PHÖNIX	Captopril	19124-f01-369346	2
PHÖNIX	Captopril	19124-f01-63946	1
Phönix	Captopril	2100156002	1
Phönix	Captopril	21003880009	1
Phönix	Captopril	22004035002	1
Sanacorp	Captopril	17077202	1
Sanacorp	Captopril	17077205	1
Sanacorp	Captopril	17210202	1
Sanacorp	Captopril	17G27B02	1
Sanacorp	Captopril	18058004	2
Sanacorp	Captopril	19/24-F01	1
Sanacorp	Captopril	190118001	2
Sanacorp	Captopril	19011806	1
Sanacorp	Captopril	19124-F01-365391	1
Sanacorp	Captopril	19124-F01-367389	3
Sonnenberg-Apotheke	Captopril	14B26-B01-291557	2
THC Pharma	Captopril	18058002	1

- 235 394 spectra from 1515 *Apo-Ident* customers from a total of 49 072 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Captopril* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

relevant spectra of the various substances were compared with *Captopril* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	620	0	201 464
Type C	0	667	6	235 394

The substance/substance group *Captopril* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.1085 % (> 98.6627 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20890	21064	6,47	145,40
21064	21064	0,00	145,19
21874	21874	0,00	145,84
21921	21874	10,51	148,93
24546	24546	0,00	142,98
25370	24546	5,38	144,22

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Carbômero**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20548-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Carbômero; Carbomera

Special notes

When selecting the *Carbômero* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Carbômero	12	23	199

Second-stage model

For differentiation of the substance/substance group *Carbômero* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Carbômero* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	46,42	42,91
Proteinato de prata	67,12	–
⋮	⋮	⋮
Fosfato de Mg-Ca-K-colamina	>50	93,52
Citrato de magnésio	>50	113,33
Sulfato de gentamicina	>50	451,79
Sulfato de tobramicina	>50	494,45
Finasterida	>50	563,77
Sulfato de neomicina	>50	609,38
Gluconato de zinco	>50	940,90
Tetraborato de sódio	>50	1068,63

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Carbômero* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Carbômero*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carbômero	13135601	20978	40	1403767
Caelo	Carbômero	13186207	20979	40	1403768
Caelo	Carbômero	14057902	21354	40	20140228
Caelo	Carbômero	14057903	21557	60	20140228
Caelo	Carbômero	162530	22759	40	20161011*
Caelo	Carbômero	21001724	25809	50	20210831*
Caelo	Carbômero	24000748	27218	40	20240419*
Euro OTC	Carbômero	1311027-02	21561	60	20131205
Euro OTC	Carbômero	1512010	22250	60	20151216*
Euro OTC	Carbômero	1604032	22548	40	20160428*
Euro OTC	Carbômero	1607028	22686	40	20160804*
Euro OTC	Carbômero	1610024	22852	40	20161102*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 12 reference samples from the substance/substance group *Carbômero*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.
- 152 412 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1040 spectra of 28 reference samples from the substance/substance group *Carbômero*.
- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Carbômero	172520	23621	40
Caelo	Carbômero	173614	23783	40
Caelo	Carbômero	180924	24250	40
Caelo	Carbômero	183074	24543	40
Caelo	Carbômero	190245	24565	40
Caelo	Carbômero	20001190	25227	40
Caelo	Carbômero	21002358	25808	50
Caelo	Carbômero	22002190	26506	40
Caelo	Carbômero	24000213	27227	40
Euro OTC	Carbômero	1702012	23139	40
Euro OTC	Carbômero	1706015	23534	40
Euro OTC	Carbômero	1801044	23959	40
Euro OTC	Carbômero	1810019	24315	40
Euro OTC	Carbômero	1903007	24468	40
Euro OTC	Carbômero	1908029	24858	40
Euro OTC	Carbômero	2003049	25124	40
Euro OTC	Carbômero	2104007	25669	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Carbômero	2112003	25915	40
Euro OTC	Carbômero	2203009	26092	40
Euro OTC	Carbômero	2206008	26195	40
Euro OTC	Carbômero	2302002	26579	40
Euro OTC	Carbômero	2310006	27010	40
Euro OTC	Carbômero	2403011	27200	40
Caelo	Carbômero	24000748	27243	40
Euro OTC	Carbômero	2112003	25915SI	10
Euro OTC	Carbômero	2203009	26092SI	20
Euro OTC	Carbômero	2206008	26195SI	20
Euro OTC	Carbômero	2302002	26579SI	20

- 201 044 spectra from a total of 4021 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 984 spectra from 565 *Apo-Ident* customers from 205 batches from the substance/substance group *Carbômero*.
- Among them are spectra of independent samples from 198 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Carbômero	22002190002	3
	Carbômero	22002190003	4
	Carbômero	23000625003	6
	Carbômero	23002015002	2
	Carbômero	23002015003	1
	Carbômero	23002015004	1
	Carbômero	2302002-01	3
	Carbômero	24000213002	1
Alliance H.	Carbômero	1512010-01	1
Alliance Healthcare	Carbômero	21001724008	1
Anzag	Carbômero	23000625003	1
apo ident	Carbômero	2003049-01	1
Bombastus	Carbômero	18092401	1
Bombastus	Carbômero	22002190003	1
Caeli/sana	Carbômero	21003605001	1
Caelo	Carbômero	10003550042	1
Caelo	Carbômero	1081702	1
Caelo	Carbômero	11013605	2
Caelo	Carbômero	1117I-01232	1
Caelo	Carbômero	11307511	1
Caelo	Carbômero	11351604	1
Caelo	Carbômero	11351605	3
Caelo	Carbômero	11351618	3
Caelo	Carbômero	11351623	1
Caelo	Carbômero	11676321	1
Caelo	Carbômero	12274907	7
Caelo	Carbômero	12274908	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carbômero	12274910	1
Caelo	Carbômero	12274912	5
Caelo	Carbômero	12274914	3
Caelo	Carbômero	12274916	8
Caelo	Carbômero	12274922	1
Caelo	Carbômero	1311027-02	1
Caelo	Carbômero	13186201	2
Caelo	Carbômero	13186203	3
Caelo	Carbômero	13186205	6
Caelo	Carbômero	13186207	1
Caelo	Carbômero	13194501	5
Caelo	Carbômero	13194503	7
Caelo	Carbômero	13194505	2
Caelo	Carbômero	13194507	4
Caelo	Carbômero	13194511	1
Caelo	Carbômero	13194512	1
Caelo	Carbômero	14016208	7
Caelo	Carbômero	14016209	1
Caelo	Carbômero	14057902	2
Caelo	Carbômero	14057903	2
Caelo	Carbômero	1410001-02	1
Caelo	Carbômero	14149904	2
Caelo	Carbômero	14149905	1
Caelo	Carbômero	14149906	4
Caelo	Carbômero	14149910	2
Caelo	Carbômero	14149911	2
Caelo	Carbômero	15015702	1
Caelo	Carbômero	15015703	1
Caelo	Carbômero	15015709	2
Caelo	Carbômero	15101801	5
Caelo	Carbômero	15101802	6
Caelo	Carbômero	15101807	3
Caelo	Carbômero	15101809	4
Caelo	Carbômero	15101810	5
Caelo	Carbômero	1510801	1
Caelo	Carbômero	15257401	1
Caelo	Carbômero	15257403	1
Caelo	Carbômero	154390002	1
Caelo	Carbômero	15439002	12
Caelo	Carbômero	15439003	11
Caelo	Carbômero	15439004	1
Caelo	Carbômero	1604032-01	2
Caelo	Carbômero	1607028-01	1
Caelo	Carbômero	1610024-01	1
Caelo	Carbômero	162375	1
Caelo	Carbômero	16237501	1
Caelo	Carbômero	162530	1
Caelo	Carbômero	16253001	2
Caelo	Carbômero	16253002	1
Caelo	Carbômero	16253003	1
Caelo	Carbômero	16253004	10
Caelo	Carbômero	16253005	6
Caelo	Carbômero	16253007	10
Caelo	Carbômero	16253009	12
Caelo	Carbômero	16253011	1
Caelo	Carbômero	16253012	7
Caelo	Carbômero	16253014	5
Caelo	Carbômero	17053182	1
Caelo	Carbômero	1706015-01	1
Caelo	Carbômero	17146501	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carbômero	17361402	11
Caelo	Carbômero	17361403	5
Caelo	Carbômero	18049301	1
Caelo	Carbômero	18049304	1
Caelo	Carbômero	180924006	1
Caelo	Carbômero	18092401	37
Caelo	Carbômero	18092402	4
Caelo	Carbômero	18092403	1
Caelo	Carbômero	18092405	21
Caelo	Carbômero	18092406	6
Caelo	Carbômero	18092408	12
Caelo	Carbômero	18092411	2
Caelo	Carbômero	18092412	2
Caelo	Carbômero	1810024-01	1
Caelo	Carbômero	181016184	1
Caelo	Carbômero	18307401	18
Caelo	Carbômero	18307402	2
Caelo	Carbômero	18307403	6
Caelo	Carbômero	18307406	3
Caelo	Carbômero	18307407	1
Caelo	Carbômero	18307408	14
Caelo	Carbômero	18307410	4
Caelo	Carbômero	18307411	4
Caelo	Carbômero	18307413	2
Caelo	Carbômero	19000614002	2
Caelo	Carbômero	19000614003	1
Caelo	Carbômero	19024505	3
Caelo	Carbômero	19145601	1
Caelo	Carbômero	192276003	5
Caelo	Carbômero	192276004	18
Caelo	Carbômero	19227601	5
Caelo	Carbômero	19227602	12
Caelo	Carbômero	19236601	2
Caelo	Carbômero	2000034003	1
Caelo	Carbômero	20000343001	3
Caelo	Carbômero	20000343003	22
Caelo	Carbômero	20001190002	2
Caelo	Carbômero	20001190003	11
Caelo	Carbômero	200011910003	1
Caelo	Carbômero	2000190003	1
Caelo	Carbômero	2000190008	1
Caelo	Carbômero	20003095003	2
Caelo	Carbômero	20003238001	2
Caelo	Carbômero	20003924001	14
Caelo	Carbômero	20003924003	1
Caelo	Carbômero	20003924004	11
Caelo	Carbômero	20003929003	2
Caelo	Carbômero	210000355001	1
Caelo	Carbômero	2100035001	1
Caelo	Carbômero	21000355001	13
Caelo	Carbômero	21000355004	6
Caelo	Carbômero	21000355006	1
Caelo	Carbômero	210003605008	1
Caelo	Carbômero	21001724001	6
Caelo	Carbômero	21001724002	13
Caelo	Carbômero	21001724004	3
Caelo	Carbômero	21001724008	3
Caelo	Carbômero	21001724009	2
Caelo	Carbômero	21002358004	2
Caelo	Carbômero	21003605001	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carbômero	21003605003	8
Caelo	Carbômero	21003605008	9
Caelo	Carbômero	22002190003	7
Caelo	Carbômero	2215M-01232	1
Caelo	Carbômero	28111310	1
Caelo	Carbômero	2913M1232	1
Caelo	Carbômero	3000034003	1
Caelo	Carbômero	31631293	1
Caelo	Carbômero	3441	1
Caelo	Carbômero	42(20003924001)	1
Caelo	Carbômero	9011903	1
Caeol	Carbômero	16253004	1
Caesar & Loretz GmbH…	Carbômero	21001724008	1
Caesar & Loretz GmbH…	Carbômero	23000179002	1
Caesar & Loretz GmbH…	Carbômero	19227601	1
Caesar & Loretz GmbH…	Carbômero	21003605003	3
Caesar & Loretz GmbH…	Carbômero	19236601	1
Caesar & Loretz GmbH…	Carbômero	20000343003	1
Caesar & Loretz GmbH…	Carbômero	20003924004	1
Caesar & Loretz GmbH…	Carbômero	21001724002	1
Caesar & Loretz GmbH/Gehe	Carbômero	21001724001	1
Caesar & Loretz GmbH…	Carbômero	21001724001	1
Caesar & Loretz GmbH…	Carbômero	22002190003	1
Caesar & Loretz GmbH/Kehr	Carbômero	18307411	1
Caesar & Loretz GmbH/Kehr	Carbômero	20001190003	1
Caesar & Loretz GmbH/Kehr	Carbômero	21001724001	1
Caesar & Loretz GmbH…	Carbômero	19227601	1
Caesar & Loretz GmbH/L10	Carbômero	20001190003	1
Caesar & Loretz GmbH…	Carbômero	20003095003	1
Caesar & Loretz GmbH…	Carbômero	21001724008	1
Caesar & Loretz GmbH…	Carbômero	20003924004	1
Caesar & Loretz GmbH…	Carbômero	20003924004	2
Caesar & Loretz GmbH…	Carbômero	21000355001	1
Caesar & Loretz GmbH…	Carbômero	21000355004	1
Caesar & Loretz GmbH…	Carbômero	18307406	1
Caesar & Loretz GmbH…	Carbômero	18307410	1
Caesar & Loretz GmbH…	Carbômero	20003095003	1
Caesar & Loretz GmbH…	Carbômero	21000355001	1
Caesar & Loretz GmbH…	Carbômero	21003605008	1
Caesar & Loretz GmbH…	Carbômero	19227601	1
Caesar & Loretz GmbH…	Carbômero	21001724001	1
Caesar & Loretz GmbH…	Carbômero	19227602	1
Caesar & Loretz GmbH	Carbômero	18092401	2
Caesar & Loretz GmbH	Carbômero	18092405	1
Caesar & Loretz GmbH	Carbômero	18092406	1
Caesar & Loretz GmbH	Carbômero	18092408	1
Caesar & Loretz GmbH	Carbômero	18092412	1
Caesar & Loretz GmbH	Carbômero	18307401	1
Caesar & Loretz GmbH	Carbômero	18307402	1
Caesar & Loretz GmbH	Carbômero	18307406	2
Caesar & Loretz GmbH	Carbômero	18307407	3
Caesar & Loretz GmbH	Carbômero	18307408	1
Caesar & Loretz GmbH	Carbômero	18307410	3
Caesar & Loretz GmbH	Carbômero	18307411	2
Caesar & Loretz GmbH	Carbômero	19024501	1
Caesar & Loretz GmbH	Carbômero	19024505	1
Caesar & Loretz GmbH	Carbômero	1903007-01	1
Caesar & Loretz GmbH	Carbômero	192276004	4
Caesar & Loretz GmbH	Carbômero	192276005	1
Caesar & Loretz GmbH	Carbômero	19227602	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Carbômero	19227603	1
Caesar & Loretz GmbH	Carbômero	20000343001	2
Caesar & Loretz GmbH	Carbômero	20000343003	4
Caesar & Loretz GmbH	Carbômero	20001190003	7
Caesar & Loretz GmbH	Carbômero	20001190007	1
Caesar & Loretz GmbH	Carbômero	20001190008	2
Caesar & Loretz GmbH	Carbômero	20003095003	1
Caesar & Loretz GmbH	Carbômero	20003924001	6
Caesar & Loretz GmbH	Carbômero	20003924004	7
Caesar & Loretz GmbH	Carbômero	21000355001	1
Caesar & Loretz GmbH	Carbômero	21000355002	1
Caesar & Loretz GmbH	Carbômero	21000355004	6
Caesar & Loretz GmbH	Carbômero	21001724001	2
Caesar & Loretz GmbH	Carbômero	21001724002	2
Caesar & Loretz GmbH	Carbômero	21001724008	8
Caesar & Loretz GmbH	Carbômero	21003605001	2
Caesar & Loretz GmbH	Carbômero	21003605003	3
Caesar & Loretz GmbH	Carbômero	21003605008	3
Caesar & Loretz GmbH	Carbômero	22002070002	1
Caesar & Loretz GmbH	Carbômero	22002190003	4
Caesar & Loretz Hild…	Carbômero	18307403	1
Caesar & Loretz/Geil…	Carbômero	20000343003	1
Caesar & Loretz	Carbômero	18092408	1
Caesar & Loretz	Carbômero	18307408	1
Caesar&Loretz,Phönix…	Carbômero	15439003	1
Caesar/Phönix	Carbômero	21001724008	1
Cealo	Carbômero	18307408	1
Cordes/Phönix	Carbômero	192276004	1
Eu Rho	Carbômero	2203009-01	1
EuRho/ Noweda	Carbômero	1908029-01	1
EuRho/ Phönix	Carbômero	2003049-01	1
EuRho	Carbômero	1210037-01	1
EuRho	Carbômero	1311027-02	1
EuRho	Carbômero	1410001-01	2
Euro OTC	Carbômero		1
Euro OTC	Carbômero	101217279	1
Euro OTC	Carbômero	101616773	2
Euro OTC	Carbômero	102026590	1
Euro OTC	Carbômero	102540805	1
Euro OTC	Carbômero	120202001	2
Euro OTC	Carbômero	1202020-01	2
Euro OTC	Carbômero	12052014A	1
Euro OTC	Carbômero	1210037-01	6
Euro OTC	Carbômero	1305007-01	2
Euro OTC	Carbômero	130800601	1
Euro OTC	Carbômero	1311027-01	3
Euro OTC	Carbômero	1311027-02	7
Euro OTC	Carbômero	141000-01	1
Euro OTC	Carbômero	141000101	1
Euro OTC	Carbômero	1410001-01	13
Euro OTC	Carbômero	1512010-01	8
Euro OTC	Carbômero	1512010-02	5
Euro OTC	Carbômero	151210-02	1
Euro OTC	Carbômero	1518E2	1
Euro OTC	Carbômero	1604032-01	8
Euro OTC	Carbômero	1607028-01	10
Euro OTC	Carbômero	1610024-01	21
Euro OTC	Carbômero	16253002	1
Euro OTC	Carbômero	16253014	1
Euro OTC	Carbômero	1702012-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Carbômero	1706015-01	4
Euro OTC	Carbômero	17361402	1
Euro OTC	Carbômero	18010019-01	1
Euro OTC	Carbômero	1801044-01	6
Euro OTC	Carbômero	1810019-01	10
Euro OTC	Carbômero	18307401	1
Euro OTC	Carbômero	190300-01	1
Euro OTC	Carbômero	1903007-01	5
Euro OTC	Carbômero	1908029-01	3
Euro OTC	Carbômero	2003049-01	8
Euro OTC	Carbômero	210400701	1
Euro OTC	Carbômero	2104007-01	5
Euro OTC	Carbômero	2112003-01	1
Euro OTC	Carbômero	2203009-01	1
Euro OTC	Carbômero	2206008-01	4
Euro OTC	Carbômero	41(1810019-01)	1
Euro OTC	Carbômero	4311027-01	1
Euro/Gehe	Carbômero	1604032-01	1
Euro/Phönix	Carbômero	161002401	1
Euro/Sanacorp	Carbômero	1305007-01	1
Euro	Carbômero	1410001-01	2
Fagron	Carbômero	13194503	1
Fagron	Carbômero	1607028-01	1
Fiebig	Carbômero	2003049-01	1
Fischer/Gehe	Carbômero	1410001-02	1
Gatt-Koller	Carbômero	1800201	1
Gehe 04.11.21 EK:7,78EUR	Carbômero	211105CM	1
Gehe	Carbômero	102669851	1
Gehe	Carbômero	13194505	1
Gehe	Carbômero	16237501	1
GEHE	Carbômero	18092405	1
Gehe	Carbômero	18307408	1
Gehe	Carbômero	22002190003	1
Gehe	Carbômero	2302002-01	1
Hepart AG	Carbômero	12274916	1
Ichthyol/Phönix	Carbômero	14149905	1
Jenne	Carbômero	18049301	2
Kehr	Carbômero	23000685003	1
L10/apo-ident	Carbômero	1512010-01	1
L30	Carbômero	1610024-01	1
L30	Carbômero	1801044-01	2
Nachtestung	Carbômero		1
Noweda Taucha	Carbômero	21001724008	1
Noweda/ Caesar&Loren…	Carbômero	192276004	1
Noweda	Carbômero	16253012	1
Noweda	Carbômero	20000343003	1
Noweda	Carbômero	21000355004	1
Noweda	Carbômero	22002190003	1
Noweda	Carbômero	2206008-01	1
Noweda	Carbômero	23000823003	1
Pharbil Waltrop GmbH	Carbômero	102237289	4
Pharbil Waltrop GmbH	Carbômero	102246780	1
Phoenix 16.04.2014	Carbômero	13194503	1
Phoenix	Carbômero	18307402	1
Phoenix	Carbômero	19227602	1
Phoenix	Carbômero	20003924003	1
Phönix Gotha	Carbômero	19227601	1
Phönix	Carbômero	18092405	1
Phönix	Carbômero	18092411	1
Phönix	Carbômero	200011980008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
PHÖNIX	Carbômero	21000355004	2
Phönix	Carbômero	22002190003	1
Rezepturlager - Verl…	Carbômero	115/14	1
Sanacaorp	Carbômero	14149905	1
Sanacorp	Carbômero	12274922	1
Sanacorp	Carbômero	1311027-01	1
Sanacorp	Carbômero	14149911	1
Sanacorp	Carbômero	1604032-01	1
Sanacorp	Carbômero	160702801	1
Sanacorp	Carbômero	18307411	1
Sanacorp	Carbômero	19227601	1
Sanacorp	Carbômero	20003924004	1
Sanacorp	Carbômero	20003929003	2
sanacorp	Carbômero	22002190002	1
Sanacorp	Carbômero	2302002-01	1
Sanacorp	Carbômero	6/AKD13	1

- 235 083 spectra from 1515 *Apo-Ident* customers from a total of 49 056 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Carbômero* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Carbômero* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	550	0	152 412
Type B	0	1040	0	201 044
Type C	0	982	2	235 083

The substance/substance group *Carbômero* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9091 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4231 %)
Type C	100.0000 % (> 99.9007 %)	99.7967 % (> 99.4919 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20978	20978	0,00	116,86
20979	20979	0,00	103,64
21354	22852	12,61	115,19
21557	22686	13,45	118,89
21561	22548	6,98	109,92
22250	22250	0,00	112,84
22548	22548	0,00	106,27
22686	22686	0,00	110,10
22759	22759	0,00	181,28
22852	22852	0,00	104,84
25809	25809	0,00	194,16
27218	27218	0,00	121,14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Carmelose sódica**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20866-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Carmelose sódica; Carboximetilcelulose sódica; Carmellosum natricum; CMC-Na

Special notes

When selecting the *Carmelose sódica* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Carmelose sódica	10	6	70

Second-stage model

For differentiation of the substance/substance group *Carmelose sódica* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Carmelose sódica* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	53,50	–
⋮	⋮	⋮
SyrSpend® SF Alka	>50	21,75
SyrSpend® SF pH4 neo	>50	26,25
Sulfato de colistina	>50	33,59
Glicerofosfato de cálcio	>50	38,38
Amido de milho	>50	38,90
Amido de arroz	>50	39,18
Sulfato de polimixina B	65,97	39,41
Goma arábica, dispersão seca	>50	39,81
Anfotericina B	>50	45,90
Bacitracina	>50	46,57
Cianocobalamina	>50	48,46
Amido de trigo	>50	48,69
SyrSpend® SF pH4	>50	51,61
Levedura de selênio	>50	64,72
Riboflavina	>50	66,20
Maltodextrina	>50	71,01
Fécula de batata	>50	74,59
Nistatina	>50	82,85
Tosilcloramida sódica	>50	89,37
Ácido oxálico	>50	90,75
Pantotenato de cálcio	>50	101,23
Vitamina E acetato pó 50%	>50	112,68
Gelatina, branca	>50	113,39
Estradiol hemi-hidratado	>50	114,13
Bromidrato de hioscina	>50	121,13
Estriol	>50	127,98
Triancinolona	>50	149,47
Frutose	>50	176,93
Metilcobalamina	>50	195,43

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Carmelose sódica* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Carmelose sódica*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carmelose sódica	12354404	20866	40	1401185
Caelo	Carmelose sódica	13104807	20872	40	1401186
Caelo	Carmelose sódica	14029211	21382	40	20140127
Caelo	Carmelose sódica	13299310	21432	60	20131002
Caelo	Carmelose sódica	161714	22645	40	20160713*
Caelo	Carmelose sódica	16171406	23187	40	AR-17-FG-015964-01
Caelo	Carmelose sódica	180486	24039	40	20180228*
Caelo	Carmelose sódica	22002555	26352	40	20220922*
Caelo	Carmelose sódica	22002555	26352SI	20	20220922*
Fagron	Carmelose sódica	13D22-N02	20892	40	1401187
Fagron	Carmelose sódica	18E15-B04-354617	24868	40	20180620

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Carmelose sódica*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 522 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Carmelose sódica*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Carmelose sódica	17062304	23519	40
Caelo	Carmelose sódica	172446	23623	40
Caelo	Carmelose sódica	20000171001	25500	40
Caelo	Carmelose sódica	22000132008	26311	30
Caelo	Carmelose sódica	23000402	26712	40
Caelo	Carmelose sódica	23001501	26844	40
Caelo	Carmelose sódica	22000132008	26311SI	20
Caelo	Carmelose sódica	23000402	26712SI	20

- 201 814 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 218 spectra from 132 *Apo-Ident* customers from 73 batches from the substance/substance group *Carmelose sódica*.
- Among them are spectra of independent samples from 70 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Carmelose sódica	22000132001	1
	Carmelose sódica	23000402001	2
	Carmelose sódica	23000402002	6
	Carmelose sódica	23000402005	4
	Carmelose sódica	23001501001	1
Alliance Healthcare	Carmelose sódica	21000062004	2
Bombastus	Carmelose sódica	13104813	1
Caelo	Carmelose sódica	10000620042	1
Caelo	Carmelose sódica	11124211	1
Caelo	Carmelose sódica	12255708	1
Caelo	Carmelose sódica	12354408	1
Caelo	Carmelose sódica	12354414	1
Caelo	Carmelose sódica	12354416	3
Caelo	Carmelose sódica	13104802	3
Caelo	Carmelose sódica	13104807	2
Caelo	Carmelose sódica	13104810	3
Caelo	Carmelose sódica	13104813	2
Caelo	Carmelose sódica	1315Q-03302	1
Caelo	Carmelose sódica	13299302	2
Caelo	Carmelose sódica	13G19-N02	1
Caelo	Carmelose sódica	14029201	1
Caelo	Carmelose sódica	14029211	1
Caelo	Carmelose sódica	14149806	2
Caelo	Carmelose sódica	15123901	5
Caelo	Carmelose sódica	15123908	5
Caelo	Carmelose sódica	15123909	1
Caelo	Carmelose sódica	15123912	1
Caelo	Carmelose sódica	16171402	3
Caelo	Carmelose sódica	17052304	1
Caelo	Carmelose sódica	17062303	2
Caelo	Carmelose sódica	17062304	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carmelose sódica	17062307	5
Caelo	Carmelose sódica	17062308	2
Caelo	Carmelose sódica	17062309	3
Caelo	Carmelose sódica	17244601	2
Caelo	Carmelose sódica	17348601	8
Caelo	Carmelose sódica	17348604	1
Caelo	Carmelose sódica	17348605	7
Caelo	Carmelose sódica	17348606	1
Caelo	Carmelose sódica	180486003	8
Caelo	Carmelose sódica	18048602	2
Caelo	Carmelose sódica	18048604	11
Caelo	Carmelose sódica	18048607	1
Caelo	Carmelose sódica	2000132001	1
Caelo	Carmelose sódica	20001837002	5
Caelo	Carmelose sódica	21000062003	1
Caelo	Carmelose sódica	21000062004	6
Caelo	Carmelose sódica	21000062007	2
Caelo	Carmelose sódica	2119M-04170	1
Caelo	Carmelose sódica	218U-03302	1
Caelo	Carmelose sódica	22000132001	4
Caelo	Carmelose sódica	22000132002	2
Caelo	Carmelose sódica	22000132009	2
Caelo	Carmelose sódica	22002555003	2
Caelo	Carmelose sódica	22002555005	1
Caelo	Carmelose sódica	22002555006	2
Caelo	Carmelose sódica	22002555007	2
Caelo	Carmelose sódica	23000402002	5
Caelo	Carmelose sódica	23000402005	1
Caelo	Carmelose sódica	25041805	1
Caelo	Carmelose sódica	28051402	1
Caelo	Carmelose sódica	36/17	1
Caesar & Loretz GmbH...	Carmelose sódica	17244601	1
Caesar & Loretz GmbH...	Carmelose sódica	18048604	1
Caesar & Loretz GmbH...	Carmelose sódica	22002555007	1
Caesar & Loretz GmbH...	Carmelose sódica	18048604	1
Caesar & Loretz GmbH...	Carmelose sódica	20001837002	1
Caesar & Loretz GmbH...	Carmelose sódica	22002555006	1
Caesar & Loretz GmbH...	Carmelose sódica	18048604	1
Caesar & Loretz GmbH...	Carmelose sódica	18048604	3
Caesar & Loretz GmbH...	Carmelose sódica	23000402001	1
Caesar & Loretz GmbH	Carmelose sódica	17062307	1
Caesar & Loretz GmbH	Carmelose sódica	17348605	1
Caesar & Loretz GmbH	Carmelose sódica	18048604	3
Caesar & Loretz GmbH	Carmelose sódica	20001837002	5
Caesar & Loretz GmbH	Carmelose sódica	21000062004	1
Caesar & Loretz GmbH	Carmelose sódica	21000062007	1
Caesar & Loretz GmbH	Carmelose sódica	22000132001	1
Caesar & Loretz GmbH	Carmelose sódica	22000132002	1
Caesar & Loretz GmbH	Carmelose sódica	22000132009	2
Caesar & Loretz GmbH	Carmelose sódica	22002555003	1
Caesar & Loretz GmbH	Carmelose sódica	22002555006	2
Caesar & Loretz GmbH	Carmelose sódica	22002555007	1
Caesar & Loretz GmbH	Carmelose sódica	23000402002	3
Caesar & Loretz/AHD	Carmelose sódica	20001837002	1
Caesar&Loretz GmbH	Carmelose sódica	21000062007	1
Fagro	Carmelose sódica	15G03-B02-321790	1
Fagro	Carmelose sódica	16G05-B05-329314	1
Fagro	Carmelose sódica	17C20-B07-337104	1
Fagro	Carmelose sódica	17K06-B03-345975	1
Fagron	Carmelose sódica	13D22-N02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Carmelose sódica	15G03-B02-312862	1
Fagron	Carmelose sódica	15G03-Bo2-312862	1
Fagron	Carmelose sódica	15G03-B02-321790	1
Fagron	Carmelose sódica	7006400006	1
Gehe 06.10.14	Carmelose sódica	13299312	1
Gehe	Carmelose sódica	17062307	1
GEHE	Carmelose sódica	17062307	1
Gehe	Carmelose sódica	22000132001	1
Gutenberg-Apotheke	Carmelose sódica	4811E-03302	1
Kehr	Carmelose sódica	22000132001	1
Kehr	Carmelose sódica	22002555003	1
Kehr	Carmelose sódica	2300402005	1
Noweda	Carmelose sódica	12354401	1
Noweda	Carmelose sódica	20001837002	1
Noweda	Carmelose sódica	22002555004	1
Phoenix	Carmelose sódica	17348601	2
Phönix	Carmelose sódica	23001501005	1
Sanacorp	Carmelose sódica	180486003	1
Sanacorp	Carmelose sódica	AKD6	1

- 235 849 spectra from 1515 *Apo-Ident* customers from a total of 49 188 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Carmelose sódica* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Carmelose sódica* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	270	0	201 814
Type C	0	217	1	235 849

The substance/substance group *Carmelose sódica* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	99.5413 % (> 98.1651 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20866	20866	0,00	77,21
20872	20872	0,00	75,37
20892	20892	0,00	71,50
21382	20872	14,57	80,63
21432	20866	32,64	73,21
22645	22645	0,00	72,76
23187	23187	0,00	75,02
24039	24039	0,00	99,96
24868	20892	17,98	79,22
26352	26352	0,00	72,91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Celulose microcristalina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20708-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Celulose microcristalina; Cellulosum microcristallinum

Special notes

When selecting the *Celulose microcristalina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Celulose microcristalina	8	12	71

Second-stage model

For differentiation of the substance/substance group *Celulose microcristalina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Celulose microcristalina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	75,87	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Celulose microcristalina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Celulose microcristalina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Celulose microcristalina	1201004-01	20728	40	20120201
Euro OTC	Celulose microcristalina	1211037-01	21080	30	20121207
Euro OTC	Celulose microcristalina	1211037-01	21085	40	20121207
Euro OTC	Celulose microcristalina	1507022	21857	60	20150805*
Euro OTC	Celulose microcristalina	1604029	22559	40	20160512*
Euro OTC	Celulose microcristalina	2010026	25464	40	20201209*
Euro OTC	Celulose microcristalina	2212016	26527	40	20230112*
Euro OTC	Celulose microcristalina	2212016	26527SI	20	20230112*
Fagron	Celulose microcristalina	12C23-N06	20708	70	1403080
Fagron	Celulose microcristalina	16B24-B11-323324	22896	40	20160311

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Celulose microcristalina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 15 reference samples from the substance/substance group *Celulose microcristalina*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Celulose microcristalina	1607042	22794	40
Euro OTC	Celulose microcristalina	1604029-01	22815	40
Euro OTC	Celulose microcristalina	1610030	22876	40
Euro OTC	Celulose microcristalina	1712009	23909	40
Euro OTC	Celulose microcristalina	1811011	24346	40
Euro OTC	Celulose microcristalina	1911018	25076	40
Euro OTC	Celulose microcristalina	2005004	25248	40
Euro OTC	Celulose microcristalina	2109026	25880	50
Euro OTC	Celulose microcristalina	2309002	26938	40
Euro OTC	Celulose microcristalina	2410009	27464	40
Fagron	Celulose microcristalina	22A15-B01-217413	26293	40
Fagron	Celulose microcristalina	24A09-B01-237270	27174	40
Euro OTC	Celulose microcristalina	2109026	25880SI	10
Euro OTC	Celulose microcristalina	2309002	26938SI	20
Fagron	Celulose microcristalina	22A15-B01-217413	26293SI	20

- 201 544 spectra from a total of 4033 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 229 spectra from 152 *Apo-Ident* customers from 74 batches from the substance/substance group *Celulose microcristalina*.

- Among them are spectra of independent samples from 71 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Celulose microcristalina	2010026-01	2
	Celulose microcristalina	2109026-01	2
	Celulose microcristalina	2212016-01	4
	Celulose microcristalina	22K19-B10-224131	1
	Celulose microcristalina	2309002-01	2
	Celulose microcristalina	23L11-B04-235327	2
	Celulose microcristalina	24A09-B01-237270	1
AHD	Celulose microcristalina	2109026-1	1
Anzag	Celulose microcristalina	2005004-01	1
apo-ident.	Celulose microcristalina	1604029-01	1
apo-ident	Celulose microcristalina	1610030-01	1
Caelo	Celulose microcristalina	160402901	1
Caelo	Celulose microcristalina	1610030-01	4
Caelo	Celulose microcristalina	8722	1
DuPont	Celulose microcristalina	R0025	1
EuRho	Celulose microcristalina	1201004-02	1
Euro OTC	Celulose microcristalina	1201004-02	2
Euro OTC	Celulose microcristalina	121103701	1
Euro OTC	Celulose microcristalina	1211037-01	2
Euro OTC	Celulose microcristalina	1309001-01	3
Euro OTC	Celulose microcristalina	1309001-02	3
Euro OTC	Celulose microcristalina	135010001	1
Euro OTC	Celulose microcristalina	1410002-01	5
Euro OTC	Celulose microcristalina	1507022	1
Euro OTC	Celulose microcristalina	150702201	1
Euro OTC	Celulose microcristalina	150722-01	1
Euro OTC	Celulose microcristalina	1604029-01	10
Euro OTC	Celulose microcristalina	160704201	1
Euro OTC	Celulose microcristalina	1607042-01	3
Euro OTC	Celulose microcristalina	1610030-01	11
Euro OTC	Celulose microcristalina	1704b50351755	1
Euro OTC	Celulose microcristalina	1712009-01	2
Euro OTC	Celulose microcristalina	1712009-02	7
Euro OTC	Celulose microcristalina	1811011-01	18
Euro OTC	Celulose microcristalina	181101103	1
Euro OTC	Celulose microcristalina	1811011-03	6
Euro OTC	Celulose microcristalina	1911018-01	6
Euro OTC	Celulose microcristalina	195010861	2
Euro OTC	Celulose microcristalina	2005004-01	10
Euro OTC	Celulose microcristalina	201002601	2
Euro OTC	Celulose microcristalina	2010026-01	31
Euro OTC	Celulose microcristalina	205010638	3
Euro OTC	Celulose microcristalina	2109026-01	7
Euro OTC	Celulose microcristalina	2109026-02	3
Euro OTC	Celulose microcristalina	2763	1
Euro OTC	Celulose microcristalina	2780	1
Euro OTC	Celulose microcristalina	7/21	1
Euro OTC	Celulose microcristalina	700204	2
Euro OTC	Celulose microcristalina	8710	1
Euro OTC	Celulose microcristalina	SD17070102	2
Euro/Noweda	Celulose microcristalina	1410002-02	1
Euro/Sanacorp	Celulose microcristalina	1911018-01	1
Fagron	Celulose microcristalina	13A03-N01	1
Fagron	Celulose microcristalina	15C03-B06-305242	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Celulose microcristalina	17/04-B50	1
Fagron	Celulose microcristalina	17/04-B50-351755	1
Fagron	Celulose microcristalina	17A11-B04-331463	1
Fagron	Celulose microcristalina	17A11-B04-340541	1
Fagron	Celulose microcristalina	17I04-B50-351755	1
Fagron	Celulose microcristalina	18/19-B50-360110	2
Fagron	Celulose microcristalina	18B16-B50-355434	1
Fagron	Celulose microcristalina	18K16-B50	1
Fagron	Celulose microcristalina	18k16-b50-360224	1
Fagron	Celulose microcristalina	18K16-B50-360224	1
Fagron	Celulose microcristalina	18K16-B50-364001	1
Fagron	Celulose microcristalina	18K16-B50-364002	1
Fagron	Celulose microcristalina	18l19-B05-360110	1
Fagron	Celulose microcristalina	2005004-41	1
Fagron	Celulose microcristalina	2013M-01350	1
Fagron	Celulose microcristalina	205001122	1
Fagron	Celulose microcristalina	20E15-F03-371624	1
Fagron	Celulose microcristalina	20E15-F03-371625	1
Fagron	Celulose microcristalina	20L01-F02	1
Fagron	Celulose microcristalina	20L01-F02-376412	2
Fagron	Celulose microcristalina	20L01F02376414	2
Fagron	Celulose microcristalina	20L01-F02-376414	5
Fagron	Celulose microcristalina	23C02-B11-226149	1
Fagron	Celulose microcristalina	9K10-N10	1
Kehr	Celulose microcristalina	2212016-01	1
Koisser	Celulose microcristalina	E0790	1
Noweda	Celulose microcristalina	1811011-03	1
Noweda	Celulose microcristalina	1911018-01	1
Noweda	Celulose microcristalina	2109026-01	1
Noweda	Celulose microcristalina	2212016-01	1
Noweda	Celulose microcristalina	2215016-01	1
Phnoix	Celulose microcristalina	1211037-01	1
Phoenix	Celulose microcristalina	1309001-02	1
Phoenix	Celulose microcristalina	1712009-02	1
Phoenix	Celulose microcristalina	3235	1
ROHA	Celulose microcristalina	140010	1
Sanacorp/EuRho	Celulose microcristalina	2109026-01	1
Sanacorp	Celulose microcristalina	2005004-01	1
Sanacorp	Celulose microcristalina	2010026-01	1
Sanacorp	Celulose microcristalina	2212016-01	1

- 235 838 spectra from 1515 *Apo-Ident* customers from a total of 49 184 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Celulose microcristalina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Celulose microcristalina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	540	0	201 544
Type C	0	229	0	235 838

The substance/substance group *Celulose microcristalina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.3799 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20708	20708	0,00	119,62
20728	20708	9,57	121,37
21080	20708	8,74	118,71
21085	20708	8,43	119,61
21857	21857	0,00	115,20
22559	22559	0,00	117,57
22896	21857	7,63	116,00
25464	25464	0,00	118,42
26527	26527	0,00	112,93

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ceras/gorduras**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20865-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ceras/gorduras; Adeps solidus; Adeps solidus W35; Base para supositório (Witepsol W35); Cera alba; Cera de abelha, amarela; Cera de abelha, branca; Cera flava; Cetylis palmitas; Dodecilsulfato de sódio; Gordura sólida; Hard fat W35; Lauril sulfato de sódio; Manteiga de cacau; Natrii laurilsulfas; Palmitato de cetila; Paraffina microcristallina; Paraffinum solidum; Parafina sólida; Parafina, microcristalina; Theobromatis oleum

Special notes

When selecting the *Ceras/gorduras* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ceras/gorduras	59	49	1135

Second-stage model

For differentiation of the substance/substance group *Ceras/gorduras* the following second-stage model is used:

- Submodelo 01

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ceras/gorduras* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estearato de magnésio	67,37	21,80

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ceras/gorduras* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ceras/gorduras*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Base para supositório (Wi...	15A07-B12-302751	21880	60	1604639
Fagron	Base para supositório (Wi...	15A07-B12-309245	22338	60	20150115
Fagron	Base para supositório (Wi...	16K08-B10-334910	23601	40	20161229
Fagron	Base para supositório (Wi...	19C04-B09-191420	25047	40	20190330
Fagron	Base para supositório (Wi...	20H17-B09-202675	25445	40	20200904
Fagron	Base para supositório (Wi...	23G27-B04-231463	27034	40	20230830
Bombastus	Cera de abelha, amarela	23002495	26910	40	20230530
Caelo	Cera de abelha, amarela	13335507	21433	60	20131011
Caelo	Cera de abelha, amarela	15317602	22245	60	20151007
Caelo	Cera de abelha, amarela	21004132003	26734	40	20220128
Caelo	Cera de abelha, amarela	21004132003	26734SI	20	20220128
Klenk	Cera de abelha, amarela	0290A170314	23511	40	1908177
Klenk	Cera de abelha, amarela	0290A170915	24870	40	20190507
Caelo	Cera de abelha, branca	13378619	21483	20	1509364
Caelo	Cera de abelha, branca	14336620	22244	60	20141125
Caelo	Cera de abelha, branca	15292022	22956	40	20150827
Caelo	Cera de abelha, branca	20003825001	25739	50	20201123
Caelo	Cera de abelha, branca	22000795006	26622	40	20220329
Fagron	Cera de abelha, branca	21C26-B07-204255	25723	50	2110141
Fagron	Cera de abelha, branca	23I12-B02-233063	27268	40	20230927
Fagron	Cera de abelha, branca	23I12-B02-233063	27268SI	20	20230927
Caelo	Dodecilsulfato de sódio	13099011	20986	40	1403108

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dodecilsulfato de sódio	15344503	22352	60	20151022
Caelo	Dodecilsulfato de sódio	16229217	23242	40	20160809
Caelo	Dodecilsulfato de sódio	170955	23278	40	20170503*
Caelo	Dodecilsulfato de sódio	191243	24715	40	20190521*
Caelo	Dodecilsulfato de sódio	190923	24716	40	20190521*
Caelo	Dodecilsulfato de sódio	20001260	25216	40	20200512*
Caelo	Dodecilsulfato de sódio	22000409	26108	40	20220427*
Caelo	Dodecilsulfato de sódio	22000409	26108SI	20	20220427*
Caelo	Dodecilsulfato de sódio	23000156	26696	40	20230209*
Caelo	Dodecilsulfato de sódio	23000156	26696SI	20	20230209*
Bombastus	Gordura sólida	306363	23565	34	20161213
Bombastus	Gordura sólida	308558	23705	40	20170321
Bombastus	Gordura sólida	20002467	25381	40	20200518
Caelo	Gordura sólida	12158122	21067	40	20120627
Caelo	Gordura sólida	160278	22479	60	20160407*
Caelo	Gordura sólida	20003131	25639	40	20201210*
Caelo	Gordura sólida	22002076	26362	40	20220805*
Caelo	Manteiga de cacau	13292013	21482	40	20130924
Caelo	Manteiga de cacau	14348906	22348	60	20150122
Caelo	Manteiga de cacau	163165	23067	40	20161116*
Caelo	Manteiga de cacau	17055907	23707	33	20170310
Caelo	Manteiga de cacau	190360	24813	40	20190227*
Caelo	Manteiga de cacau	19000676008	25384	40	20200318
Caelo	Palmitato de cetila	12331916	20865	40	1402429
Caelo	Palmitato de cetila	14351606	21875	60	20141219
Caelo	Palmitato de cetila	15301703	21984	60	AR-16-FG-007435-01
Caelo	Palmitato de cetila	15301703	22325	60	20151013
Caelo	Palmitato de cetila	160538	22486	60	20160323*
Caelo	Palmitato de cetila	17043503	23560	40	20170306
Caelo	Palmitato de cetila	171640	23639	40	20170719*
Caelo	Palmitato de cetila	172715	23817	40	20171124*
Caelo	Palmitato de cetila	191390	24720	40	20190702*
Caelo	Palmitato de cetila	23001428	26959	40	20231108*
Caelo	Parafina sólida	13390413	21731	60	20131213
Caelo	Parafina sólida	15232004	22349	60	1702507
Caelo	Parafina sólida	192463001	25387	40	20191024
Caelo	Parafina sólida	21001748	26745	40	20210701
Caelo	Parafina sólida	21001748	26745SI	20	20210701
Caelo	Parafina, microcristalina	14307104	21682	60	AR-15-FG-005277-01
Caelo	Parafina, microcristalina	14307106	21766	60	20141014
Caelo	Parafina, microcristalina	154128	22330	60	20160112*
Caelo	Parafina, microcristalina	19234501	25434	40	20191015
Caelo	Parafina, microcristalina	23003019	27418	40	20240126*
Caelo	Parafina, microcristalina	23003019	27418SI	20	20240126*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2847 spectra of 66 reference samples from the substance/substance group *Ceras/gorduras*. These samples are listed above in the *calibration samples* section. The reference samples come from 59 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 150 115 spectra from a total of 2783 batches from further 477 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2203 spectra of 63 reference samples from the substance/substance group *Ceras/gorduras*.
- Among them are spectra of independent samples from 49 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Base para supositório (Wi…	15J08-B04-324959	22806	40
Fagron	Base para supositório (Wi…	17K09-B03-343779	24114	40
Fagron	Base para supositório (Wi…	20J07-B02-202717	25748	50
Fagron	Base para supositório (Wi…	21B23-B98-211232	25908	40
Bombastus	Cera de abelha, amarela	22000930	26027	40
Caelo	Cera de abelha, amarela	162750	22767	40
Caelo	Cera de abelha, amarela	17011602	23512	40
Caelo	Cera de abelha, amarela	20003602005	25738	50
Caelo	Cera de abelha, amarela	23003594	27338	40
Caelo	Cera de abelha, branca	161631	22587	40
Caelo	Cera de abelha, branca	16163109	23513	40
Caelo	Cera de abelha, branca	182391	24351	40
Fagron	Cera de abelha, branca	21G17-B03-215725	26057	40
Caelo	Dodecilsulfato de sódio	13411305	21465	60
Caelo	Dodecilsulfato de sódio	16229205	23243	40
Caelo	Dodecilsulfato de sódio	172363	23664	40
Caelo	Dodecilsulfato de sódio	181822	24292	40
Caelo	Dodecilsulfato de sódio	190187	24549	40
Caelo	Dodecilsulfato de sódio	20001952	25222	40
Caelo	Dodecilsulfato de sódio	24001699	27333	40
Bombastus	Gordura sólida	18006248	24663	40
Bombastus	Gordura sólida	21004219	26026	40
Bombastus	Gordura sólida	23001364	26623	40
Caelo	Gordura sólida	173076	23814	40
Caelo	Gordura sólida	181479	24228	40
Caelo	Gordura sólida	183339	24529	40
Caelo	Gordura sólida	191940	24887	40
Caelo	Gordura sólida	21003046	25846	50
Caelo	Gordura sólida	23000561	26700	35
Caelo	Gordura sólida	23001036	27120	40
Caelo	Gordura sólida	24001755	27450	40
Euro OTC	Gordura sólida	2303007	26674	40
Euro OTC	Gordura sólida	2307014	26920	40
Caelo	Manteiga de cacau	173149	23795	40
Caelo	Manteiga de cacau	181351	24226	40

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Manteiga de cacau	182544	24363	40
Caelo	Manteiga de cacau	21002516002	25934	40
Caelo	Manteiga de cacau	23001467	27106	40
Caelo	Palmitato de cetila	13295919	21316	20
Caelo	Palmitato de cetila	181499	24221	40
Caelo	Palmitato de cetila	182737	24356	40
Caelo	Palmitato de cetila	192859	25224	40
Caelo	Palmitato de cetila	21000860001	25933	40
Caelo	Palmitato de cetila	22000395002	26411	40
Caelo	Palmitato de cetila	24001934	27451	40
Caelo	Parafina sólida	16277704	23190	40
Caelo	Parafina sólida	23003232	27416	40
Caelo	Parafina, microcristalina	15412801	23724	40
Caelo	Parafina, microcristalina	21003773006	26237	35
Bombastus	Cera de abelha, amarela	22000930	26027SI	10
Bombastus	Cera de abelha, amarela	23002495	26910SI†	20
Caelo	Cera de abelha, branca	22000795006	26622SI†	20
Fagron	Cera de abelha, branca	21G17-B03-215725	26057SI	10
Caelo	Dodecilsulfato de sódio	24001699	27333SI	20
Bombastus	Gordura sólida	306363	23565†	6
Bombastus	Gordura sólida	21004219	26026SI	10
Caelo	Manteiga de cacau	17055907	23707†	7
Caelo	Palmitato de cetila	13295919	21522	40
Caelo	Palmitato de cetila	21000860001	25933SI	10
Caelo	Palmitato de cetila	23001428	26959SI†	20
Caelo	Palmitato de cetila	24001934	27451SI	20
Caelo	Parafina sólida	23003232	27416SI	20
Caelo	Parafina, microcristalina	21003773006	26237SI	10

- 199 881 spectra from a total of 3991 batches from further 834 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5726 spectra from 992 *Apo-Ident* customers from 1111 batches from the substance/substance group *Ceras/gorduras*.

- Among them are spectra of independent samples from 1063 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Manteiga de cacau	18254412	1
	Cera de abelha, amarela	20000280008	1
	Cera de abelha, branca	20000885007	1
	Gordura sólida	20003131003	1
	Cera de abelha, amarela	20003602009	1
	Palmitato de cetila	20003842013	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Cera de abelha, branca	21001267002	1
	Cera de abelha, branca	21001267008	1
	Cera de abelha, branca	21001267012	2
	Cera de abelha, amarela	21001423003	3
	Cera de abelha, amarela	21001423010	3
	Parafina sólida	2100174018	1
	Parafina sólida	21001748004	1
	Parafina sólida	21001748012	2
	Parafina sólida	21001748014	3
	Parafina sólida	21001748017	1
	Parafina sólida	21001748018	8
	Manteiga de cacau	21002516020	2
	Gordura sólida	21003046011	1
	Cera de abelha, amarela	21004132003	14
	Cera de abelha, amarela	21004132004	4
	Cera de abelha, branca	22000795001	6
	Cera de abelha, branca	22000795006	4
	Cera de abelha, branca	22000795007	6
	Palmitato de cetila	220017004	1
	Palmitato de cetila	22001717001	1
	Palmitato de cetila	22001717004	4
	Palmitato de cetila	22001785003	4
	Gordura sólida	22002076002	1
	Gordura sólida	22002076008	1
	Gordura sólida	22002076010	1
	Base para supositório (Wi...	22002377	1
	Manteiga de cacau	22003120004	4
	Manteiga de cacau	22003120014	1
	Cera de abelha, branca	22003630003	4
	Cera de abelha, amarela	22003888002	7
	Palmitato de cetila	2201717001	1
	Base para supositório (Wi...	22J26-B12-224506	1
	Dodecilsulfato de sódio	23000156006	1
	Dodecilsulfato de sódio	23000156007	1
	Gordura sólida	23000447	3
	Gordura sólida	23000561002	16
	Gordura sólida	23000561003	1
	Gordura sólida	23000561006	1
	Gordura sólida	23000561008	2
	Gordura sólida	23001036004	1
	Parafina sólida	23001089003	1
	Gordura sólida	23001364	4
	Palmitato de cetila	23001428006	11
	Manteiga de cacau	23001467004	2
	Manteiga de cacau	23001467005	3
	Cera de abelha, branca	23002638006	1
	Parafina sólida	23003232004	1
	Parafina sólida	23003232005	1
	Cera de abelha, amarela	23003298002	1
	Gordura sólida	2300561002	1
	Cera de abelha, amarela	230120-001	1
	Cera de abelha, amarela	230413-001	3
	Palmitato de cetila	24000124003	1
	Cera de abelha, branca	280A22111501	1
	Cera de abelha, branca	280A221115-01	3
	Cera de abelha, branca	280A230413-01	1
	Cera de abelha, branca	280A230413-02	2
	Cera de abelha, amarela	290A230120-01	4
	Cera de abelha, amarela	290A230413-01	6
	Cera de abelha, amarela	30413-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Manteiga de cacau	423300201	1
	Cera de abelha, branca	42374	2
	Cera de abelha, amarela	44064	1
/ AHD	Manteiga de cacau	20004174002	1
ACM	Manteiga de cacau	KNC1605J15	1
aep	Cera de abelha, amarela	21001423010	1
AHC	Cera de abelha, amarela	21001423003	1
AHC	Parafina sólida	23003232005	1
AHD	Manteiga de cacau	14348906	1
AHD	Cera de abelha, amarela	15022908	1
AHD	Cera de abelha, amarela	18299202	1
AHD	Cera de abelha, branca	22000795001	1
AHD	Cera de abelha, branca	22000795006	1
AHD	Palmitato de cetila	22001785003	1
AHD	Manteiga de cacau	22003120004	1
AHD	Cera de abelha, amarela	22003888002	1
AHD	Gordura sólida	23000561002	1
AHD	Palmitato de cetila	23001428006	2
AHD	Cera de abelha, amarela	23003298002	1
AHD	Gordura sólida	277212	2
Alliance H.	Palmitato de cetila	15301709	1
Alliance Health 14.0…	Cera de abelha, amarela	280A130115	1
Alliance Healthcare	Palmitato de cetila	13131905	1
Alliance Healthcare	Cera de abelha, amarela	290A120627	1
Alliance Healthcare	Cera de abelha, branca	5443200038243	1
Alliance	Parafina sólida	21001748018	1
Alliance	Cera de abelha, amarela	21004132003	1
Alliance	Palmitato de cetila	22001785003	1
Alliance	Cera de abelha, amarela	280A130115	1
Anzag	Manteiga de cacau	11117816	1
Anzag	Palmitato de cetila	12018208	1
Anzag	Manteiga de cacau	12342004	1
Anzag	Cera de abelha, amarela	1462	1
Anzag	Parafina sólida	21000732001	1
Anzag	Cera de abelha, amarela	23003298002	1
Anzag	Parafina sólida	42241	1
apomix	Manteiga de cacau	1017300203	1
apomix	Gordura sólida	18147901	1
Bambastus/Gehe	Base para supositório (Wi…	18006248	1
Beiersdorf	Cera de abelha, branca	15292014	1
BOM	Base para supositório (Wi…	22004876	1
Bombastus	Cera de abelha, branca	16163109	1
Bombastus	Cera de abelha, amarela	17011604	1
Bombastus	Gordura sólida	17107304	2
Bombastus	Cera de abelha, amarela	17207405	1
Bombastus	Manteiga de cacau	17314901	1
Bombastus	Gordura sólida	18000345	1
Bombastus	Gordura sólida	18000346	6
Bombastus	Gordura sólida	18004024	6
Bombastus	Gordura sólida	18006248	3
Bombastus	Gordura sólida	19001444	1
Bombastus	Gordura sólida	19001445	3
Bombastus	Gordura sólida	19002628	1
Bombastus	Gordura sólida	19002629	2
Bombastus	Gordura sólida	20000603	7
Bombastus	Gordura sólida	20002467	7
Bombastus	Base para supositório (Wi…	20005051	2
Bombastus	Gordura sólida	21004219	2
Bombastus	Gordura sólida	22002377	8
Bombastus	Gordura sólida	22004876	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Gordura sólida	23000447	3
Bombastus	Cera de abelha, amarela	267702	1
Bombastus	Cera de abelha, amarela	270682	3
Bombastus	Gordura sólida	273759	1
Bombastus	Cera de abelha, amarela	279999	1
Bombastus	Cera de abelha, branca	280A171019	1
Bombastus	Cera de abelha, amarela	285109	1
Bombastus	Gordura sólida	287287	1
Bombastus	Cera de abelha, amarela	290A170915	1
Bombastus	Cera de abelha, amarela	292025	1
Bombastus	Gordura sólida	293848	7
Bombastus	Cera de abelha, amarela	296261	1
Bombastus	Gordura sólida	302709	3
Bombastus	Gordura sólida	306363	5
Bombastus	Gordura sólida	308559	3
Bombastus	Cera de abelha, amarela	caelo	1
Bombstus/Geilenkirchen	Base para supositório (Wi…	18004024	1
cae	Cera de abelha, amarela	15317608	1
Cae4lo	Gordura sólida	15185002	1
Caele	Cera de abelha, amarela	17011607	1
Caelo	Cera de abelha, amarela		9
Caelo	Cera de abelha, branca	10023025	1
Caelo	Palmitato de cetila	10068410	1
Caelo	Cera de abelha, amarela	10121302	1
Caelo	Gordura sólida	10158813	1
Caelo	Manteiga de cacau	1018302053	1
Caelo	Parafina sólida	10194101	2
Caelo	Manteiga de cacau	103276705	1
Caelo	Cera de abelha, amarela	10364810	1
Caelo	Cera de abelha, amarela	10364837	1
Caelo	Cera de abelha, branca	10651388	1
Caelo	Cera de abelha, amarela	11017308	1
Caelo	Cera de abelha, amarela	11017314	1
Caelo	Cera de abelha, amarela	11017315	1
Caelo	Cera de abelha, amarela	11017318	3
Caelo	Parafina sólida	11021202	1
Caelo	Palmitato de cetila	11021502	1
Caelo	Manteiga de cacau	11034718	1
Caelo	Manteiga de cacau	11034719	1
Caelo	Palmitato de cetila	11042019	1
Caelo	Gordura sólida	11109617	1
Caelo	Gordura sólida	11109623	2
Caelo	Manteiga de cacau	11117816	1
Caelo	Dodecilsulfato de sódio	11220208	1
Caelo	Cera de abelha, amarela	11285001	2
Caelo	Cera de abelha, amarela	11285014	2
Caelo	Cera de abelha, amarela	11285015	1
Caelo	Cera de abelha, amarela	11308305	1
Caelo	Cera de abelha, amarela	11308311	2
Caelo	Gordura sólida	11345904	1
Caelo	Gordura sólida	11345905	3
Caelo	Gordura sólida	11345917	3
Caelo	Gordura sólida	11345918	7
Caelo	Gordura sólida	1135917	1
Caelo	Parafina sólida	1136206	1
Caelo	Parafina sólida	11363205	1
Caelo	Parafina sólida	11363206	2
Caelo	Parafina sólida	11363220	3
Caelo	Palmitato de cetila	12018204	3
Caelo	Palmitato de cetila	12018204/Int212191	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Palmitato de cetila	12018208	6
Caelo	Palmitato de cetila	12018215	1
Caelo	Manteiga de cacau	12040802	1
Caelo	Manteiga de cacau	12040803	1
Caelo	Manteiga de cacau	12040807	2
Caelo	Cera de abelha, amarela	12041303	1
Caelo	Palmitato de cetila	12082901	1
Caelo	Cera de abelha, amarela	12091404	1
Caelo	Parafina, microcristalina	12095101	1
Caelo	Gordura sólida	12111204	1
Caelo	Cera de abelha, amarela	12124801	4
Caelo	Cera de abelha, amarela	12124802	2
Caelo	Cera de abelha, amarela	121248024-2015	1
Caelo	Cera de abelha, amarela	12124805	4
Caelo	Cera de abelha, amarela	12124806	2
Caelo	Cera de abelha, amarela	12124807	3
Caelo	Cera de abelha, amarela	12124810	4
Caelo	Cera de abelha, amarela	12124811	1
Caelo	Cera de abelha, amarela	12124812	8
Caelo	Cera de abelha, amarela	12124814	2
Caelo	Cera de abelha, amarela	12124816	1
Caelo	Cera de abelha, amarela	12124817	2
Caelo	Cera de abelha, amarela	1214816	1
Caelo	Dodecilsulfato de sódio	12153003	1
Caelo	Dodecilsulfato de sódio	12153004	1
Caelo	Dodecilsulfato de sódio	12153010	3
Caelo	Dodecilsulfato de sódio	12153019	1
Caelo	Gordura sólida	12158104	5
Caelo	Gordura sólida	12158109	3
Caelo	Gordura sólida	12158114	3
Caelo	Gordura sólida	12158115	6
Caelo	Gordura sólida	12158119	1
Caelo	Gordura sólida	12158122	1
Caelo	Palmitato de cetila	122228801/Int212191	1
Caelo	Palmitato de cetila	12228805	1
Caelo	Palmitato de cetila	12228808	3
Caelo	Palmitato de cetila	12228818	5
Caelo	Parafina sólida	12252205	2
Caelo	Parafina sólida	12252206	1
Caelo	Parafina sólida	12252211	3
Caelo	Parafina sólida	12252221	3
Caelo	Cera de abelha, branca	122570	1
Caelo	Cera de abelha, amarela	12257002	3
Caelo	Cera de abelha, amarela	12257004	2
Caelo	Cera de abelha, amarela	12257009	7
Caelo	Cera de abelha, amarela	12257012	3
Caelo	Cera de abelha, amarela	12257022	3
Caelo	Manteiga de cacau	12270201	2
Caelo	Manteiga de cacau	12270202	4
Caelo	Manteiga de cacau	12270203	4
Caelo	Manteiga de cacau	12270209	2
Caelo	Manteiga de cacau	12270210	2
Caelo	Palmitato de cetila	1228808	1
Caelo	Cera de abelha, amarela	12330116	1
Caelo	Palmitato de cetila	12331916	8
Caelo	Palmitato de cetila	12331919	2
Caelo	Manteiga de cacau	12342003	7
Caelo	Manteiga de cacau	12342004	2
Caelo	Parafina, microcristalina	12355001	1
Caelo	Parafina sólida	123654	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	12367020	1
Caelo	Cera de abelha, amarela	12367901	12
Caelo	Cera de abelha, amarela	12367904	5
Caelo	Cera de abelha, amarela	12367910	11
Caelo	Cera de abelha, amarela	12367911	2
Caelo	Cera de abelha, amarela	12367912	3
Caelo	Cera de abelha, amarela	12367915	8
Caelo	Cera de abelha, amarela	12367916	6
Caelo	Cera de abelha, amarela	12367916-3429311150	1
Caelo	Cera de abelha, amarela	12367921	1
Caelo	Gordura sólida	12K01-N12	2
Caelo	Cera de abelha, amarela	12K20B05287421	1
Caelo	Dodecilsulfato de sódio	13014604	2
Caelo	Manteiga de cacau	13027202	4
Caelo	Manteiga de cacau	13027203	1
Caelo	Manteiga de cacau	13027204	4
Caelo	Manteiga de cacau	13027207	1
Caelo	Manteiga de cacau	13027221	4
Caelo	Manteiga de cacau	13027224	5
Caelo	Manteiga de cacau	13027226	4
Caelo	Manteiga de cacau	13027227	3
Caelo	Cera de abelha, amarela	13031201	4
Caelo	Cera de abelha, amarela	13031206	8
Caelo	Cera de abelha, amarela	13031220	3
Caelo	Cera de abelha, amarela	13031221	1
Caelo	Cera de abelha, amarela	13031222	3
Caelo	Cera de abelha, amarela	13031231	6
Caelo	Cera de abelha, amarela	13031239	11
Caelo	Cera de abelha, amarela	13051401	1
Caelo	Cera de abelha, amarela	13061503	1
Caelo	Dodecilsulfato de sódio	13099006	3
Caelo	Dodecilsulfato de sódio	13099011	3
Caelo	Parafina sólida	13109203	4
Caelo	Parafina sólida	13109213	6
Caelo	Parafina sólida	13109214	4
Caelo	Parafina sólida	13109218	1
Caelo	Parafina sólida	13109221	1
Caelo	Parafina sólida	13109224	4
Caelo	Palmitato de cetila	1313190	1
Caelo	Palmitato de cetila	13131905	3
Caelo	Palmitato de cetila	13131905NP	1
Caelo	Palmitato de cetila	13131906	8
Caelo	Palmitato de cetila	13131911	2
Caelo	Palmitato de cetila	13131914	4
Caelo	Manteiga de cacau	13140401	1
Caelo	Manteiga de cacau	13140404	2
Caelo	Manteiga de cacau	13140405	3
Caelo	Manteiga de cacau	13140406	3
Caelo	Manteiga de cacau	13140407	3
Caelo	Manteiga de cacau	13140409	1
Caelo	Gordura sólida	13243301	5
Caelo	Gordura sólida	13243403	8
Caelo	Gordura sólida	13243409	5
Caelo	Gordura sólida	13243411	3
Caelo	Gordura sólida	13243412	2
Caelo	Gordura sólida	13243414	1
Caelo	Gordura sólida	13243416	1
Caelo	Gordura sólida	13243418	3
Caelo	Gordura sólida	13243419	3
Caelo	Gordura sólida	13243420	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Parafina, microcristalina	13274301	1
Caelo	Parafina, microcristalina	13274303	5
Caelo	Manteiga de cacau	13292001	2
Caelo	Manteiga de cacau	13292006	4
Caelo	Manteiga de cacau	13292007	9
Caelo	Manteiga de cacau	13292011	2
Caelo	Manteiga de cacau	13292012	3
Caelo	Manteiga de cacau	13292013	9
Caelo	Manteiga de cacau	13292015	1
Caelo	Manteiga de cacau	13292019	3
Caelo	Palmitato de cetila	13295910	8
Caelo	Palmitato de cetila	13295919	10
Caelo	Palmitato de cetila	13295921	1
Caelo	Cera de abelha, amarela	133335507	1
Caelo	Cera de abelha, amarela	13335502	9
Caelo	Cera de abelha, amarela	13335503	6
Caelo	Cera de abelha, amarela	13335505	1
Caelo	Cera de abelha, amarela	13335507	6
Caelo	Cera de abelha, amarela	13335508	1
Caelo	Cera de abelha, amarela	13335509	2
Caelo	Cera de abelha, amarela	13335513	3
Caelo	Cera de abelha, amarela	13335516	1
Caelo	Cera de abelha, amarela	13335517	4
Caelo	Cera de abelha, amarela	13335518	2
Caelo	Cera de abelha, amarela	1335503	1
Caelo	Cera de abelha, amarela	13378602	1
Caelo	Cera de abelha, amarela	13378603	1
Caelo	Cera de abelha, amarela	13378619	13
Caelo	Cera de abelha, amarela	13378630	2
Caelo	Cera de abelha, amarela	13378634	6
Caelo	Cera de abelha, amarela	13378636	1
Caelo	Cera de abelha, amarela	13378639	3
Caelo	Cera de abelha, amarela	13378640	3
Caelo	Parafina sólida	13390403	1
Caelo	Parafina sólida	13390406	4
Caelo	Parafina sólida	13390408	1
Caelo	Parafina sólida	13390413	1
Caelo	Parafina sólida	13390415	3
Caelo	Dodecilsulfato de sódio	13411302	2
Caelo	Dodecilsulfato de sódio	13411304	1
Caelo	Dodecilsulfato de sódio	13411305	3
Caelo	Manteiga de cacau	1392013	1
Caelo	Palmitato de cetila	14041505	1
Caelo	Manteiga de cacau	14045104	1
Caelo	Palmitato de cetila	14060705	6
Caelo	Palmitato de cetila	14060706	6
Caelo	Palmitato de cetila	14060709	6
Caelo	Manteiga de cacau	14123609	2
Caelo	Manteiga de cacau	14123611	6
Caelo	Manteiga de cacau	14123617	4
Caelo	Manteiga de cacau	14123620	6
Caelo	Manteiga de cacau	14123621	1
Caelo	Gordura sólida	1412602	1
Caelo	Gordura sólida	14126202	5
Caelo	Gordura sólida	14126203	7
Caelo	Gordura sólida	14126204	2
Caelo	Gordura sólida	14126205	1
Caelo	Gordura sólida	14126210	3
Caelo	Gordura sólida	14126216	2
Caelo	Gordura sólida	14126217	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Gordura sólida	14126218	2
Caelo	Dodecilsulfato de sódio	14127406	3
Caelo	Dodecilsulfato de sódio	14127411	1
Caelo	Cera de abelha, amarela	1418915	1
Caelo	Cera de abelha, amarela	14189901	1
Caelo	Cera de abelha, amarela	14189902	2
Caelo	Cera de abelha, amarela	14189905	3
Caelo	Cera de abelha, amarela	14189906	1
Caelo	Cera de abelha, amarela	14189907	2
Caelo	Cera de abelha, amarela	14189908	1
Caelo	Cera de abelha, amarela	14189909	5
Caelo	Cera de abelha, amarela	14189912	6
Caelo	Cera de abelha, amarela	14189913	2
Caelo	Cera de abelha, amarela	14189914	4
Caelo	Cera de abelha, amarela	14189915	2
Caelo	Cera de abelha, amarela	14189917	3
Caelo	Cera de abelha, amarela	14189919	2
Caelo	Cera de abelha, amarela	14189920	1
Caelo	Palmitato de cetila	14213705	3
Caelo	Palmitato de cetila	14213706	1
Caelo	Palmitato de cetila	14213709	4
Caelo	Palmitato de cetila	14213710	2
Caelo	Palmitato de cetila	142137710	1
Caelo	Dodecilsulfato de sódio	14224206	1
Caelo	Dodecilsulfato de sódio	14283904	3
Caelo	Parafina sólida	14286502	1
Caelo	Parafina sólida	14286503	1
Caelo	Parafina sólida	14286504	1
Caelo	Parafina sólida	14286511	2
Caelo	Parafina sólida	14286517	4
Caelo	Manteiga de cacau	14304703	1
Caelo	Parafina, microcristalina	14307108	2
Caelo	Parafina, microcristalina	14307110	1
Caelo	Cera de abelha, amarela	14336605	3
Caelo	Cera de abelha, amarela	14336607	11
Caelo	Cera de abelha, amarela	14336608	3
Caelo	Cera de abelha, amarela	14336609	2
Caelo	Cera de abelha, amarela	14336616	11
Caelo	Cera de abelha, amarela	14336617	1
Caelo	Cera de abelha, amarela	14336618	1
Caelo	Cera de abelha, amarela	14336620	8
Caelo	Cera de abelha, branca	14336621	1
Caelo	Gordura sólida	14338703	3
Caelo	Gordura sólida	14338704	4
Caelo	Gordura sólida	14338705	1
Caelo	Gordura sólida	14338706	1
Caelo	Gordura sólida	14338707	3
Caelo	Gordura sólida	14338708	1
Caelo	Gordura sólida	14338711	2
Caelo	Manteiga de cacau	14348906	9
Caelo	Manteiga de cacau	14348908	2
Caelo	Manteiga de cacau	14348909	2
Caelo	Palmitato de cetila	14351601	2
Caelo	Palmitato de cetila	14351602	5
Caelo	Palmitato de cetila	14351606	4
Caelo	Palmitato de cetila	14351607	1
Caelo	Palmitato de cetila	14351609	3
Caelo	Palmitato de cetila	14351612	15
Caelo	Palmitato de cetila	14351614	1
Caelo	Cera de abelha, amarela	1436607	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	1436616	1
Caelo	Cera de abelha, amarela	1436620	1
Caelo	Cera de abelha, amarela	14G07-B04-300495	1
Caelo	Cera de abelha, amarela	15022902	7
Caelo	Cera de abelha, amarela	15022904	4
Caelo	Cera de abelha, amarela	15022907	1
Caelo	Cera de abelha, amarela	15022908	9
Caelo	Cera de abelha, amarela	15023003	5
Caelo	Cera de abelha, amarela	15023004	9
Caelo	Cera de abelha, amarela	15023006	3
Caelo	Cera de abelha, amarela	15041301	1
Caelo	Cera de abelha, amarela	150622CF	1
Caelo	Manteiga de cacau	15088903	1
Caelo	Manteiga de cacau	15088904	1
Caelo	Manteiga de cacau	15088905	1
Caelo	Dodecilsulfato de sódio	15095404	1
Caelo	Cera de abelha, amarela	15098901	1
Caelo	Cera de abelha, amarela	15098902	1
Caelo	Gordura sólida	15111402	1
Caelo	Dodecilsulfato de sódio	15119907	4
Caelo	Cera de abelha, branca	151210CA	1
Caelo	Gordura sólida	15185002	17
Caelo	Gordura sólida	15185003	11
Caelo	Gordura sólida	15185005	15
Caelo	Gordura sólida	15185007	2
Caelo	Gordura sólida	15185009	10
Caelo	Gordura sólida	1518505	1
Caelo	Parafina sólida	1523002	1
Caelo	Parafina sólida	152320004	1
Caelo	Parafina sólida	15232001	1
Caelo	Parafina sólida	15232004	8
Caelo	Manteiga de cacau	15246102	6
Caelo	Cera de abelha, branca	1529003	1
Caelo	Cera de abelha, amarela	152920004	1
Caelo	Cera de abelha, branca	15292002	1
Caelo	Cera de abelha, amarela	15292003	9
Caelo	Cera de abelha, amarela	15292004	14
Caelo	Cera de abelha, amarela	15292005	7
Caelo	Cera de abelha, amarela	15292007	1
Caelo	Cera de abelha, amarela	15292009	4
Caelo	Cera de abelha, branca	15292010	1
Caelo	Cera de abelha, branca	15292011	1
Caelo	Cera de abelha, amarela	15292014	26
Caelo	Cera de abelha, branca	15292015	1
Caelo	Cera de abelha, amarela	15292022	10
Caelo	Cera de abelha, branca	15292023	1
Caelo	Parafina sólida	15295405	5
Caelo	Parafina sólida	15295406	3
Caelo	Parafina sólida	15295407	2
Caelo	Parafina sólida	15295410	4
Caelo	Parafina sólida	15295414	3
Caelo	Palmitato de cetila	15301701	7
Caelo	Palmitato de cetila	15301703	11
Caelo	Palmitato de cetila	15301704	6
Caelo	Palmitato de cetila	15301705	8
Caelo	Palmitato de cetila	15301708	1
Caelo	Palmitato de cetila	15301709	5
Caelo	Palmitato de cetila	15301711	7
Caelo	Cera de abelha, amarela	15317601	8
Caelo	Cera de abelha, amarela	15317602	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	15317603	3
Caelo	Cera de abelha, amarela	15317607	10
Caelo	Cera de abelha, amarela	15317608	8
Caelo	Cera de abelha, amarela	15317609	12
Caelo	Cera de abelha, amarela	15317610	6
Caelo	Cera de abelha, amarela	15317611	1
Caelo	Cera de abelha, amarela	15317613	8
Caelo	Dodecilsulfato de sódio	15344503	5
Caelo	Dodecilsulfato de sódio	15344505	2
Caelo	Dodecilsulfato de sódio	15344510	7
Caelo	Dodecilsulfato de sódio	15344511	1
Caelo	Dodecilsulfato de sódio	15344515	2
Caelo	Parafina, microcristalina	15412801	2
Caelo	Parafina, microcristalina	15412808	1
Caelo	Palmitato de cetila	15632	1
Caelo	Cera de abelha, amarela	1595	1
Caelo	Parafina sólida	16000903	3
Caelo	Parafina sólida	16000910	2
Caelo	Parafina, microcristalina	16000911	5
Caelo	Parafina sólida	16000912	5
Caelo	Parafina sólida	16000921	4
Caelo	Parafina sólida	16000922	3
Caelo	Gordura sólida	16021503	1
Caelo	Gordura sólida	16027801	6
Caelo	Gordura sólida	16027802	7
Caelo	Gordura sólida	16027805	4
Caelo	Gordura sólida	16027806	1
Caelo	Cera de abelha, amarela	16034206	1
Caelo	Cera de abelha, amarela	16038201	21
Caelo	Cera de abelha, amarela	16038202	19
Caelo	Cera de abelha, amarela	16038203	10
Caelo	Cera de abelha, amarela	16038205	2
Caelo	Cera de abelha, amarela	16038206	22
Caelo	Cera de abelha, amarela	16038207	10
Caelo	Cera de abelha, amarela	16038210	5
Caelo	Manteiga de cacau	16049201	4
Caelo	Manteiga de cacau	16049209	2
Caelo	Cera de abelha, amarela	16051702	1
Caelo	Palmitato de cetila	16053803	9
Caelo	Palmitato de cetila	16053804	1
Caelo	Palmitato de cetila	16053805	2
Caelo	Palmitato de cetila	16053811	8
Caelo	Manteiga de cacau	16062602	1
Caelo	Manteiga de cacau	16062604	1
Caelo	Cera de abelha, amarela	161202CF/15317611	1
Caelo	Cera de abelha, branca	16163101	1
Caelo	Cera de abelha, branca	16163105	36
Caelo	Cera de abelha, branca	16163106	1
Caelo	Cera de abelha, branca	16163109	21
Caelo	Cera de abelha, amarela	16163112	2
Caelo	Cera de abelha, amarela	16163114	26
Caelo	Cera de abelha, branca	16163115	3
Caelo	Palmitato de cetila	16186805	17
Caelo	Palmitato de cetila	16186806	1
Caelo	Palmitato de cetila	16186809	18
Caelo	Dodecilsulfato de sódio	16229205	6
Caelo	Dodecilsulfato de sódio	16229206	4
Caelo	Dodecilsulfato de sódio	16229209	1
Caelo	Dodecilsulfato de sódio	16229213	2
Caelo	Dodecilsulfato de sódio	16229217	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dodecilsulfato de sódio	16229218	1
Caelo	Dodecilsulfato de sódio	16229220	3
Caelo	Base para supositório (Wi…	16271201	1
Caelo	Gordura sólida	16274201	15
Caelo	Gordura sólida	16274202	1
Caelo	Gordura sólida	16274203	16
Caelo	Gordura sólida	16274205	3
Caelo	Gordura sólida	16274207	1
Caelo	Gordura sólida	16274208	18
Caelo	Parafina sólida	16277704	6
Caelo	Parafina sólida	16277705	3
Caelo	Parafina sólida	16277706	6
Caelo	Parafina sólida	16277710	3
Caelo	Parafina sólida	16277714	1
Caelo	Parafina sólida	16277716	1
Caelo	Manteiga de cacau	163116508	1
Caelo	Manteiga de cacau	16315602	1
Caelo	Manteiga de cacau	16316501	4
Caelo	Manteiga de cacau	16316503	6
Caelo	Manteiga de cacau	16316508	26
Caelo	Manteiga de cacau	16316509	5
Caelo	Manteiga de cacau	163316508	1
Caelo	Base para supositório (Wi…	16K08-B10	1
Caelo	Parafina sólida	17(21000732001)	1
Caelo	Cera de abelha, amarela	170011602	1
Caelo	Cera de abelha, amarela	170011607	2
Caelo	Cera de abelha, amarela	17011403	1
Caelo	Cera de abelha, amarela	17011602	14
Caelo	Cera de abelha, amarela	17011604	10
Caelo	Cera de abelha, amarela	17011605	1
Caelo	Cera de abelha, amarela	17011607	14
Caelo	Cera de abelha, amarela	17011609	9
Caelo	Cera de abelha, amarela	17011610	2
Caelo	Cera de abelha, amarela	17011611	11
Caelo	Cera de abelha, amarela	17011612	30
Caelo	Cera de abelha, amarela	17011619	1
Caelo	Cera de abelha, amarela	1701607	1
Caelo	Cera de abelha, amarela	1701611	1
Caelo	Gordura sólida	17041401	1
Caelo	Cera de abelha, amarela	17041402	1
Caelo	Palmitato de cetila	17043503	11
Caelo	Palmitato de cetila	17043504	11
Caelo	Palmitato de cetila	17043509	1
Caelo	Manteiga de cacau	170555901	1
Caelo	Manteiga de cacau	17055902	12
Caelo	Manteiga de cacau	17055905	1
Caelo	Manteiga de cacau	17055907	17
Caelo	Manteiga de cacau	17055908	8
Caelo	Manteiga de cacau	17055913	1
Caelo	Parafina sólida	1706989	1
Caelo	Cera de abelha, branca	17091802	37
Caelo	Cera de abelha, branca	17091803	7
Caelo	Gordura sólida	170921AS/16274208	1
Caelo	Dodecilsulfato de sódio	17095504	8
Caelo	Dodecilsulfato de sódio	17095505	1
Caelo	Dodecilsulfato de sódio	17095511	13
Caelo	Gordura sólida	17107301	8
Caelo	Gordura sólida	17107304	12
Caelo	Gordura sólida	17107305	1
Caelo	Gordura sólida	17107306	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	17121201	1
Caelo	Cera de abelha, amarela	17121202	1
Caelo	Parafina, microcristalina	17137502	1
Caelo	Palmitato de cetila	17164004	19
Caelo	Palmitato de cetila	17164005	19
Caelo	Palmitato de cetila	17164007	1
Caelo	Cera de abelha, amarela	172007402	1
Caelo	Cera de abelha, amarela	17207402	24
Caelo	Cera de abelha, amarela	17207403	13
Caelo	Cera de abelha, amarela	17207404	2
Caelo	Cera de abelha, amarela	17207405	1
Caelo	Dodecilsulfato de sódio	17236302	1
Caelo	Parafina sólida	17245602	14
Caelo	Parafina sólida	17245604	1
Caelo	Palmitato de cetila	17271502	8
Caelo	Palmitato de cetila	17271502P-180920-3	1
Caelo	Palmitato de cetila	17271502P-181227-7	1
Caelo	Palmitato de cetila	17271504	14
Caelo	Palmitato de cetila	17271505	16
Caelo	Palmitato de cetila	17271506	1
Caelo	Gordura sólida	17307601	37
Caelo	Gordura sólida	17307602	9
Caelo	Gordura sólida	17307603	1
Caelo	Gordura sólida	17307604	1
Caelo	Gordura sólida	17307607	2
Caelo	Gordura sólida	1730765	1
Caelo	Manteiga de cacau	17314901	4
Caelo	Manteiga de cacau	17314902	31
Caelo	Parafina sólida	1734701	1
Caelo	Parafina sólida	17347701	24
Caelo	Gordura sólida	18040401	17
Caelo	Gordura sólida	18040401P-181227-5	1
Caelo	Dodecilsulfato de sódio	18045202	2
Caelo	Dodecilsulfato de sódio	18045203	1
Caelo	Cera de abelha, branca	18048901	46
Caelo	Cera de abelha, branca	18048903	6
Caelo	Cera de abelha, branca	18048904	1
Caelo	Cera de abelha, branca	18048904P-181227-1	1
Caelo	Cera de abelha, amarela	18048906	40
Caelo	Cera de abelha, branca	18048907	6
Caelo	Cera de abelha, amarela	18049001	29
Caelo	Cera de abelha, amarela	18049002	3
Caelo	Cera de abelha, amarela	18049003	8
Caelo	Parafina sólida	18070103P-181227-2	1
Caelo	Parafina sólida	18070107	30
Caelo	Parafina sólida	18070110P-190624-3	1
Caelo	Gordura sólida	18070112	14
Caelo	Parafina sólida	18070118	17
Caelo	Parafina sólida	18070130P-200217-5	1
Caelo	Parafina sólida	18070131	31
Caelo	Cera de abelha, branca	180748901	1
Caelo	Cera de abelha, amarela	18113501	42
Caelo	Cera de abelha, amarela	18113502	6
Caelo	Cera de abelha, amarela	18113503	1
Caelo	Cera de abelha, amarela	18113505	47
Caelo	Cera de abelha, amarela	18113506	13
Caelo	Cera de abelha, amarela	18113507	1
Caelo	Cera de abelha, amarela	18113507P-191022-6	1
Caelo	Cera de abelha, amarela	18113507P-200102-2	1
Caelo	Cera de abelha, amarela	18113509	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	18121201	1
Caelo	Dodecilsulfato de sódio	1812207	1
Caelo	Manteiga de cacau	18135101	1
Caelo	Manteiga de cacau	18135102	3
Caelo	Manteiga de cacau	18135106	4
Caelo	Manteiga de cacau	18135107	1
Caelo	Manteiga de cacau	18135112	7
Caelo	Gordura sólida	18147901	7
Caelo	Gordura sólida	18147902	32
Caelo	Gordura sólida	18147905	2
Caelo	Gordura sólida	18147907	3
Caelo	Gordura sólida	18147908	10
Caelo	Palmitato de cetila	181499004	1
Caelo	Palmitato de cetila	18149902	4
Caelo	Palmitato de cetila	18149904	23
Caelo	Palmitato de cetila	18149911	5
Caelo	Palmitato de cetila	18149911P-190405-3	1
Caelo	Palmitato de cetila	18149911P-190718-9	1
Caelo	Palmitato de cetila	18149912	17
Caelo	Dodecilsulfato de sódio	18182206	6
Caelo	Dodecilsulfato de sódio	18182207	1
Caelo	Dodecilsulfato de sódio	18182216	1
Caelo	Cera de abelha, branca	18239102	34
Caelo	Cera de abelha, branca	18239104	7
Caelo	Cera de abelha, branca	18239106	28
Caelo	Cera de abelha, branca	18239107	4
Caelo	Cera de abelha, branca	18239108	1
Caelo	Cera de abelha, branca	18239108P-191206-5	1
Caelo	Cera de abelha, branca	18239108P-200217-4	1
Caelo	Cera de abelha, branca	18239108P-200609-6	1
Caelo	Manteiga de cacau	18254402	2
Caelo	Manteiga de cacau	18254412	6
Caelo	Palmitato de cetila	18273704	21
Caelo	Palmitato de cetila	18273705	3
Caelo	Palmitato de cetila	18273709P-191022-5	1
Caelo	Palmitato de cetila	18273709P-200102-3	1
Caelo	Palmitato de cetila	182737704	1
Caelo	Cera de abelha, amarela	18299201	13
Caelo	Cera de abelha, amarela	18299202	7
Caelo	Cera de abelha, amarela	18299206	1
Caelo	Cera de abelha, amarela	18299208	16
Caelo	Cera de abelha, amarela	18299210	3
Caelo	Gordura sólida	18333903	1
Caelo	Gordura sólida	18333904	17
Caelo	Gordura sólida	18333905	28
Caelo	Base para supositório (Wi…	18333906	1
Caelo	Gordura sólida	18333908	1
Caelo	Gordura sólida	1833905	1
Caelo	Base para supositório (Wi…	18G13-B02-356977	1
Caelo	Manteiga de cacau	19000676001	1
Caelo	Manteiga de cacau	19000676007	2
Caelo	Manteiga de cacau	19000676008	4
Caelo	Manteiga de cacau	19000676010	1
Caelo	Manteiga de cacau	19000676011	5
Caelo	Dodecilsulfato de sódio	19018702	1
Caelo	Dodecilsulfato de sódio	19018704	3
Caelo	Palmitato de cetila	1902859003	1
Caelo	Cera de abelha, amarela	19031810	1
Caelo	Manteiga de cacau	190360009	5
Caelo	Manteiga de cacau	190360010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manteiga de cacau	19036003	5
Caelo	Manteiga de cacau	19036006	1
Caelo	Manteiga de cacau	19036007	3
Caelo	Manteiga de cacau	19036008	6
Caelo	Cera de abelha, amarela	19041704	1
Caelo	Dodecilsulfato de sódio	19075403	1
Caelo	Palmitato de cetila	190902a	1
Caelo	Dodecilsulfato de sódio	190923001	2
Caelo	Palmitato de cetila	19121803	1
Caelo	Cera de abelha, branca	191242001	7
Caelo	Cera de abelha, branca	191242004	21
Caelo	Cera de abelha, amarela	19124202	30
Caelo	Cera de abelha, branca	19124203	2
Caelo	Cera de abelha, branca	19124206	31
Caelo	Cera de abelha, branca	19124207	3
Caelo	Cera de abelha, branca	19124208	1
Caelo	Cera de abelha, branca	19124210	21
Caelo	Cera de abelha, branca	19124211	4
Caelo	Cera de abelha, amarela	191372001	29
Caelo	Cera de abelha, amarela	191372002	1
Caelo	Cera de abelha, amarela	191372003	1
Caelo	Cera de abelha, amarela	19137201	5
Caelo	Cera de abelha, amarela	19137202	35
Caelo	Cera de abelha, amarela	19137206	23
Caelo	Palmitato de cetila	19139004	35
Caelo	Palmitato de cetila	19139005	4
Caelo	Palmitato de cetila	19139005P-200206-4	1
Caelo	Palmitato de cetila	1913905	1
Caelo	Cera de abelha, amarela	1917202	1
Caelo	Gordura sólida	191940001	10
Caelo	Gordura sólida	191940002	27
Caelo	Gordura sólida	191940004	1
Caelo	Gordura sólida	191940005	8
Caelo	Gordura sólida	19194001	1
Caelo	Cera de abelha, amarela	19237202	1
Caelo	Parafina sólida	1924603010	1
Caelo	Gordura sólida	192463001	24
Caelo	Parafina sólida	192463002	1
Caelo	Parafina sólida	192463002P-200507-7	1
Caelo	Parafina sólida	192463009	1
Caelo	Parafina sólida	192463010	18
Caelo	Palmitato de cetila	192859002	7
Caelo	Palmitato de cetila	192859002P-200511-2	1
Caelo	Palmitato de cetila	192859002P-200602-2	1
Caelo	Palmitato de cetila	192859003	39
Caelo	Cera de abelha, branca	2000	1
Caelo	Cera de abelha, branca	200000885007	1
Caelo	Gordura sólida	200000906007	1
Caelo	Palmitato de cetila	200000975002	1
Caelo	Cera de abelha, amarela	20000280002	10
Caelo	Cera de abelha, amarela	20000280003	17
Caelo	Cera de abelha, amarela	20000280005	1
Caelo	Cera de abelha, amarela	20000280007	4
Caelo	Cera de abelha, amarela	20000280008	30
Caelo	Cera de abelha, amarela	2000028003	1
Caelo	Cera de abelha, amarela	2000028007	1
Caelo	Cera de abelha, amarela	2000028008	1
Caelo	Base para supositório (Wi…	200003131008	1
Caelo	Cera de abelha, branca	200003825001	1
Caelo	Manteiga de cacau	200004174002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, branca	20000885003	30
Caelo	Cera de abelha, branca	20000885004	1
Caelo	Cera de abelha, branca	20000885007	32
Caelo	Cera de abelha, branca	20000885008	8
Caelo	Gordura sólida	20000906003	14
Caelo	Gordura sólida	20000906004	7
Caelo	Gordura sólida	20000906005	2
Caelo	Gordura sólida	20000906007	14
Caelo	Palmitato de cetila	20000974002	6
Caelo	Palmitato de cetila	20000975002	17
Caelo	Dodecilsulfato de sódio	20001260003	2
Caelo	Manteiga de cacau	20001695003	14
Caelo	Manteiga de cacau	20001695004	2
Caelo	Cera de abelha, amarela	200028008	1
Caelo	Gordura sólida	20003131003	12
Caelo	Gordura sólida	20003131004	3
Caelo	Gordura sólida	20003131006	2
Caelo	Gordura sólida	20003131007	13
Caelo	Gordura sólida	20003131008	1
Caelo	Parafina sólida	2000359911	1
Caelo	Cera de abelha, amarela	20003601001	1
Caelo	Cera de abelha, amarela	20003602001	20
Caelo	Cera de abelha, amarela	20003602002	4
Caelo	Cera de abelha, amarela	20003602003	5
Caelo	Cera de abelha, amarela	20003602005	19
Caelo	Cera de abelha, amarela	20003602009	7
Caelo	Cera de abelha, amarela	2000362001	1
Caelo	Cera de abelha, branca	20003824003	5
Caelo	Cera de abelha, branca	20003825001	21
Caelo	Cera de abelha, branca	20003825005	1
Caelo	Cera de abelha, branca	2000382501	1
Caelo	Palmitato de cetila	20003842006	5
Caelo	Palmitato de cetila	20003842013	7
Caelo	Cera de abelha, branca	2000385001	2
Caelo	Manteiga de cacau	20004174002	6
Caelo	Manteiga de cacau	20004174003	1
Caelo	Manteiga de cacau	20004174009	3
Caelo	Manteiga de cacau	20004174010	5
Caelo	Cera de abelha, branca	2000885008	2
Caelo	Gordura sólida	2000906007	1
Caelo	Palmitato de cetila	2000975002	1
Caelo	Cera de abelha, amarela	20031516	1
Caelo	Cera de abelha, amarela	20031517	1
Caelo	Gordura sólida	20071501	1
Caelo	Cera de abelha, amarela	20071503	1
Caelo	Palmitato de cetila	21000359001	15
Caelo	Palmitato de cetila	2100066001	1
Caelo	Parafina sólida	21000732001	20
Caelo	Parafina sólida	21000732004	1
Caelo	Parafina sólida	21000732007	3
Caelo	Palmitato de cetila	21000860001	19
Caelo	Palmitato de cetila	21000860010	10
Caelo	Cera de abelha, branca	21001267002	14
Caelo	Cera de abelha, branca	21001267003	8
Caelo	Cera de abelha, branca	21001267008	4
Caelo	Cera de abelha, branca	21001267012	5
Caelo	Cera de abelha, branca	21001267022	1
Caelo	Cera de abelha, branca	2100127008	1
Caelo	Cera de abelha, amarela	21001423001	7
Caelo	Cera de abelha, amarela	21001423003	27

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	21001423005	9
Caelo	Cera de abelha, amarela	21001423010	12
Caelo	Cera de abelha, amarela	2100143003	1
Caelo	Parafina sólida	210017480	1
Caelo	Parafina sólida	21001748003	1
Caelo	Parafina sólida	21001748004	8
Caelo	Parafina sólida	21001748007	20
Caelo	Parafina sólida	21001748012	6
Caelo	Parafina sólida	21001748014	2
Caelo	Dodecilsulfato de sódio	21001909003	2
Caelo	Dodecilsulfato de sódio	21001909004	1
Caelo	Manteiga de cacau	21002516002	12
Caelo	Manteiga de cacau	21002516003	3
Caelo	Manteiga de cacau	21002516004	6
Caelo	Manteiga de cacau	21002516017	3
Caelo	Manteiga de cacau	21002516018	1
Caelo	Manteiga de cacau	21002516020	5
Caelo	Manteiga de cacau	21002516036	1
Caelo	Gordura sólida	21003046008	9
Caelo	Gordura sólida	21003046010	2
Caelo	Gordura sólida	21003046011	5
Caelo	Dodecilsulfato de sódio	21003606002	1
Caelo	Parafina, microcristalina	21003773004	2
Caelo	Cera de abelha, amarela	21004132003	5
Caelo	Cera de abelha, amarela	21004132004	1
Caelo	Cera de abelha, amarela	2100423003	1
Caelo	Parafina sólida	2100732001	1
Caelo	Palmitato de cetila	2100860001	1
Caelo	Palmitato de cetila	22000395002	8
Caelo	Cera de abelha, branca	22000795001	4
Caelo	Cera de abelha, branca	22000795006	10
Caelo	Palmitato de cetila	22001150003	1
Caelo	Palmitato de cetila	22001717001	1
Caelo	Palmitato de cetila	22001717004	1
Caelo	Palmitato de cetila	22001785005	1
Caelo	Gordura sólida	22002076002	7
Caelo	Gordura sólida	22002076007	2
Caelo	Gordura sólida	22002076011	1
Caelo	Manteiga de cacau	22003120014	1
Caelo	Dodecilsulfato de sódio	22003127001	2
Caelo	Cera de abelha, amarela	220425E	1
Caelo	Cera de abelha, amarela	220510/2	1
Caelo	Cera de abelha, amarela	22071301	1
Caelo	Cera de abelha, amarela	220829C	1
Caelo	Cera de abelha, branca	2271200	1
Caelo	Gordura sólida	23000561002	2
Caelo	Gordura sólida	24011302	1
Caelo	Dodecilsulfato de sódio	26031508	1
Caelo	Palmitato de cetila	26071201	1
Caelo	Cera de abelha, amarela	26091302	1
Caelo	Gordura sólida	27101703	1
Caelo	Cera de abelha, amarela	280003	1
Caelo	Cera de abelha, amarela	28011501	1
Caelo	Palmitato de cetila	28041731	1
Caelo	Cera de abelha, branca	280A150528	1
Caelo	Cera de abelha, branca	280A171019	1
Caelo	Cera de abelha, branca	280A220609-02	1
Caelo	Gordura sólida	29061803	1
Caelo	Cera de abelha, branca	29091805	1
Caelo	Cera de abelha, amarela	290A0151214	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cera de abelha, amarela	290A170915	4
Caelo	Gordura sólida	293848	1
Caelo	Cera de abelha, amarela	30011407	1
Caelo	Parafina, microcristalina	30101202	1
Caelo	Palmitato de cetila	30101301	1
Caelo	Cera de abelha, amarela	30101308	1
Caelo	Parafina sólida	302709	1
Caelo	Parafina, microcristalina	3042012M1	1
Caelo	Cera de abelha, branca	3051808	1
Caelo	Cera de abelha, amarela	3253	1
Caelo	Palmitato de cetila	3785734	1
Caelo	Cera de abelha, amarela	4031403	1
Caelo	Palmitato de cetila	43204210008601	1
Caelo	Cera de abelha, amarela	4910A-01239	1
Caelo	Cera de abelha, amarela	5022904	1
Caelo	Cera de abelha, amarela	5121707	1
Caelo	Manteiga de cacau	515A-03176	1
Caelo	Parafina, microcristalina	52622395	1
Caelo	Cera de abelha, amarela	61(20003602001)	1
Caelo	Cera de abelha, amarela	6111407	1
Caelo	Cera de abelha, amarela	7091704	1
Caelo	Gordura sólida	7101304	1
Caelo	Parafina, microcristalina	7111201	1
Caelo	Parafina, microcristalina	7111202	1
Caelo	Dodecilsulfato de sódio	720E-01907	1
Caelo	Gordura sólida	8041710	1
Caelo	Gordura sólida	8051810	1
Caelo	Gordura sólida	90915429	1
Caelo	Base para supositório (Wi…	W0000906005	2
Caesa / Alliance Hea…	Cera de abelha, branca	20003825001	1
Caesa / Alliance Hea…	Palmitato de cetila	20003842013	1
Caesar & Lorenz GmbH	Palmitato de cetila	17043504	1
Caesar & Lorenz GmbH	Palmitato de cetila	18149912	1
Caesar & Lorenz GmbH	Dodecilsulfato de sódio	18182206	1
Caesar & Lorenz GmbH	Dodecilsulfato de sódio	19018704	1
Caesar & Lorenz GmbH	Palmitato de cetila	19139004	2
Caesar & Lorenz GmbH	Palmitato de cetila	192859003	1
Caesar & Lorenz	Manteiga de cacau	13140404	1
Caesar & Lorenz	Cera de abelha, branca	20003824003	1
Caesar & Loretz GmbH…	Parafina sólida	21001748007	1
Caesar & Loretz GmbH…	Cera de abelha, amarela	15023004	1
Caesar & Loretz GmbH…	Cera de abelha, branca	15292010	1
Caesar & Loretz GmbH…	Manteiga de cacau	16316503	1
Caesar & Loretz GmbH…	Manteiga de cacau	17055908	1
Caesar & Loretz GmbH…	Cera de abelha, branca	20000885007	1
Caesar & Loretz GmbH…	Gordura sólida	191940002	1
Caesar & Loretz GmbH…	Gordura sólida	191940005	3
Caesar & Loretz GmbH…	Cera de abelha, branca	19124210	1
Caesar & Loretz GmbH…	Palmitato de cetila	192859003	1
Caesar & Loretz GmbH…	Cera de abelha, amarela	15317613	1
Caesar & Loretz GmbH…	Cera de abelha, branca	16163115	3
Caesar & Loretz GmbH…	Dodecilsulfato de sódio	16229205	1
Caesar & Loretz GmbH…	Manteiga de cacau	16316509	1
Caesar & Loretz GmbH…	Palmitato de cetila	17271505	1
Caesar & Loretz GmbH…	Cera de abelha, branca	18048907	2
Caesar & Loretz GmbH…	Cera de abelha, amarela	18049001	1
Caesar & Loretz GmbH…	Cera de abelha, amarela	18113505	1
Caesar & Loretz GmbH…	Manteiga de cacau	190360009	1
Caesar & Loretz GmbH…	Gordura sólida	20000906003	1
Caesar & Loretz GmbH…	Gordura sólida	20003131003	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Cera de abelha, amarela	21001423001	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	21004132003	1
Caesar & Loretz GmbH...	Palmitato de cetila	22000395002	1
Caesar & Loretz GmbH...	Palmitato de cetila	22001785003	1
Caesar & Loretz GmbH...	Palmitato de cetila	18149912	1
Caesar & Loretz GmbH...	Parafina sólida	18070118	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	18113509	1
Caesar & Loretz GmbH...	Palmitato de cetila	19139004	1
Caesar & Loretz GmbH...	Palmitato de cetila	192859003	1
Caesar & Loretz GmbH...	Gordura sólida	17307607	1
Caesar & Loretz GmbH...	Gordura sólida	12158104	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	11285008	1
Caesar & Loretz GmbH...	Gordura sólida	11345918	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	12367901	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	12367910	1
Caesar & Loretz GmbH...	Gordura sólida	13243403	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	18113505	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	18049001	1
Caesar & Loretz GmbH...	Gordura sólida	18333905	2
Caesar & Loretz GmbH...	Gordura sólida	18147908	1
Caesar & Loretz GmbH...	Gordura sólida	18333904	1
Caesar & Loretz GmbH...	Parafina sólida	192463010	1
Caesar & Loretz GmbH...	Manteiga de cacau	21002516002	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	20000280003	1
Caesar & Loretz GmbH...	Manteiga de cacau	18254412	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	191372001	1
Caesar & Loretz GmbH...	Parafina sólida	21000732001	1
Caesar & Loretz GmbH/ Ph	Cera de abelha, amarela	18299201	1
Caesar & Loretz GmbH...	Cera de abelha, branca	20000280008	2
Caesar & Loretz GmbH...	Cera de abelha, amarela	21001423001	2
Caesar & Loretz GmbH/AHD	Cera de abelha, amarela	19137206	1
Caesar & Loretz GmbH/AHD	Cera de abelha, branca	20003825001	2
Caesar & Loretz GmbH/AHD	Manteiga de cacau	20004174009	2
Caesar & Loretz GmbH...	Cera de abelha, amarela	20003602005	1
Caesar & Loretz GmbH...	Manteiga de cacau	20004174002	1
Caesar & Loretz GmbH...	Gordura sólida	18147908	1
Caesar & Loretz GmbH...	Gordura sólida	18333905	2
Caesar & Loretz GmbH...	Cera de abelha, branca	20000885003	1
Caesar & Loretz GmbH/E	Gordura sólida	18333904	1
Caesar & Loretz GmbH/E	Cera de abelha, branca	20000885003	1
Caesar & Loretz GmbH/E	Cera de abelha, amarela	20003602001	1
Caesar & Loretz GmbH...	Manteiga de cacau	18254402	1
Caesar & Loretz GmbH...	Gordura sólida	18333904	1
Caesar & Loretz GmbH...	Gordura sólida	18333905	1
Caesar & Loretz GmbH...	Gordura sólida	191940002	1
Caesar & Loretz GmbH...	Gordura sólida	20000906003	1
Caesar & Loretz GmbH...	Palmitato de cetila	20000975002	1
Caesar & Loretz GmbH...	Palmitato de cetila	21000359001	1
Caesar & Loretz GmbH/Gehe	Manteiga de cacau	19036003	1
Caesar & Loretz GmbH/Gehe	Cera de abelha, branca	19124206	1
Caesar & Loretz GmbH/Gehe	Cera de abelha, amarela	191372001	2
Caesar & Loretz GmbH/GEHE	Cera de abelha, amarela	19137202	1
Caesar & Loretz GmbH/Gehe	Palmitato de cetila	192859003	3
Caesar & Loretz GmbH/Gehe	Gordura sólida	20003131007	2
Caesar & Loretz GmbH/Gehe	Palmitato de cetila	20003842013	1
Caesar & Loretz GmbH...	Gordura sólida	18147908	1
Caesar & Loretz GmbH...	Cera de abelha, branca	19124206	1
Caesar & Loretz GmbH...	Cera de abelha, branca	20000885008	2
Caesar & Loretz GmbH...	Palmitato de cetila	21000359001	1
Caesar & Loretz GmbH...	Palmitato de cetila	21000860010	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Manteiga de cacau	22003120004	1
Caesar & Loretz GmbH/K	Cera de abelha, amarela	18113505	1
Caesar & Loretz GmbH/Kehr	Cera de abelha, branca	21001267012	2
Caesar & Loretz GmbH...	Cera de abelha, amarela	19137202	3
Caesar & Loretz GmbH...	Cera de abelha, amarela	19137202	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	19137206	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	20000280003	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	20000280007	1
Caesar & Loretz GmbH...	Gordura sólida	20003131003	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	20003602005	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	21001423003	1
Caesar & Loretz GmbH/PH	Palmitato de cetila	18273704	1
Caesar & Loretz GmbH/Ph	Cera de abelha, amarela	191372001	1
Caesar & Loretz GmbH/Ph	Palmitato de cetila	192859003	1
Caesar & Loretz GmbH/Ph	Cera de abelha, amarela	2000080008	1
Caesar & Loretz GmbH...	Gordura sólida	18333904	2
Caesar & Loretz GmbH...	Cera de abelha, amarela	20003602009	1
Caesar & Loretz GmbH...	Cera de abelha, branca	21001267003	2
Caesar & Loretz GmbH...	Cera de abelha, branca	21001267008	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	21001423010	1
Caesar & Loretz GmbH...	Parafina sólida	21001748007	1
Caesar & Loretz GmbH...	Parafina sólida	21001748012	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	191372001	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	19137202	1
Caesar & Loretz GmbH...	Palmitato de cetila	192859003	1
Caesar & Loretz GmbH...	Palmitato de cetila	20000974002	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	20003602001	1
Caesar & Loretz GmbH...	Gordura sólida	21003046011	2
Caesar & Loretz GmbH...	Palmitato de cetila	220001717001	1
Caesar & Loretz GmbH...	Palmitato de cetila	22001717001	1
Caesar & Loretz GmbH...	Gordura sólida	22002076002	1
Caesar & Loretz GmbH...	Gordura sólida	22002076008	1
Caesar & Loretz GmbH/Sa	Cera de abelha, branca	19124206	2
Caesar & Loretz GmbH/Sa	Palmitato de cetila	20000974002	1
Caesar & Loretz GmbH/Sa	Palmitato de cetila	20000975002	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	18113507	1
Caesar & Loretz GmbH...	Palmitato de cetila	18273704	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	18299210	1
Caesar & Loretz GmbH...	Gordura sólida	183339	1
Caesar & Loretz GmbH...	Gordura sólida	18333906	1
Caesar & Loretz GmbH...	Cera de abelha, branca	191242001	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	19137203	1
Caesar & Loretz GmbH...	Gordura sólida	19194001	1
Caesar & Loretz GmbH...	Palmitato de cetila	192859003	3
Caesar & Loretz GmbH...	Cera de abelha, amarela	20000280007	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	2000028005	1
Caesar & Loretz GmbH...	Cera de abelha, branca	20000885008	2
Caesar & Loretz GmbH...	Palmitato de cetila	20000974002	1
Caesar & Loretz GmbH...	Cera de abelha, branca	20003825001	1
Caesar & Loretz GmbH...	Palmitato de cetila	21000860009	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	21001423005	1
Caesar & Loretz GmbH...	Dodecilsulfato de sódio	21001909003	1
Caesar & Loretz GmbH...	Gordura sólida	21003046008	1
Caesar & Loretz GmbH...	Palmitato de cetila	22000395002	1
Caesar & Loretz GmbH...	Cera de abelha, branca	22000795001	1
Caesar & Loretz GmbH...	Gordura sólida	22002076001	1
Caesar & Loretz GmbH...	Cera de abelha, amarela	18113502	1
Caesar & Loretz GmbH	Palmitato de cetila	10068402	2
Caesar & Loretz GmbH	Manteiga de cacau	12270210	2
Caesar & Loretz GmbH	Cera de abelha, amarela	12367910	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cera de abelha, amarela	13031221	1
Caesar & Loretz GmbH	Cera de abelha, branca	16163105	1
Caesar & Loretz GmbH	Palmitato de cetila	16186805	1
Caesar & Loretz GmbH	Dodecilsulfato de sódio	17095504	1
Caesar & Loretz GmbH	Palmitato de cetila	17164005	1
Caesar & Loretz GmbH	Base para supositório (Wi...	17307601	1
Caesar & Loretz GmbH	Parafina sólida	17347701	1
Caesar & Loretz GmbH	Gordura sólida	18040401	1
Caesar & Loretz GmbH	Cera de abelha, branca	18048901	1
Caesar & Loretz GmbH	Cera de abelha, branca	18048906	2
Caesar & Loretz GmbH	Parafina sólida	18070107	4
Caesar & Loretz GmbH	Parafina sólida	18070110	1
Caesar & Loretz GmbH	Parafina sólida	18070112	1
Caesar & Loretz GmbH	Parafina sólida	18070118	3
Caesar & Loretz GmbH	Parafina sólida	18070130	1
Caesar & Loretz GmbH	Parafina sólida	18070131	4
Caesar & Loretz GmbH	Cera de abelha, amarela	18113502	1
Caesar & Loretz GmbH	Cera de abelha, amarela	18113505	3
Caesar & Loretz GmbH	Cera de abelha, amarela	18113506	1
Caesar & Loretz GmbH	Cera de abelha, amarela	18113509	1
Caesar & Loretz GmbH	Manteiga de cacau	18135106	2
Caesar & Loretz GmbH	Gordura sólida	18147902	2
Caesar & Loretz GmbH	Gordura sólida	18147908	1
Caesar & Loretz GmbH	Palmitato de cetila	18149904	2
Caesar & Loretz GmbH	Palmitato de cetila	18149911	1
Caesar & Loretz GmbH	Palmitato de cetila	18149912	1
Caesar & Loretz GmbH	Dodecilsulfato de sódio	18182206	1
Caesar & Loretz GmbH	Cera de abelha, branca	18239102	7
Caesar & Loretz GmbH	Cera de abelha, branca	18239104	5
Caesar & Loretz GmbH	Cera de abelha, branca	18239106	4
Caesar & Loretz GmbH	Cera de abelha, branca	18239107	2
Caesar & Loretz GmbH	Manteiga de cacau	18254402	2
Caesar & Loretz GmbH	Palmitato de cetila	18273704	10
Caesar & Loretz GmbH	Palmitato de cetila	18273705	1
Caesar & Loretz GmbH	Palmitato de cetila	18273709	2
Caesar & Loretz GmbH	Cera de abelha, amarela	18299201	1
Caesar & Loretz GmbH	Cera de abelha, amarela	18299202	2
Caesar & Loretz GmbH	Cera de abelha, amarela	18299203	1
Caesar & Loretz GmbH	Cera de abelha, amarela	18299206	2
Caesar & Loretz GmbH	Cera de abelha, amarela	18299210	1
Caesar & Loretz GmbH	Gordura sólida	18333903	2
Caesar & Loretz GmbH	Gordura sólida	18333904	3
Caesar & Loretz GmbH	Gordura sólida	18333905	9
Caesar & Loretz GmbH	Manteiga de cacau	19000676011	1
CAESAR & LORETZ GMBH	Manteiga de cacau	190360009	1
Caesar & Loretz GmbH	Manteiga de cacau	19036007	2
Caesar & Loretz GmbH	Manteiga de cacau	19036008	3
Caesar & Loretz GmbH	Manteiga de cacau	19036011	3
Caesar & Loretz GmbH	Dodecilsulfato de sódio	19075403	1
Caesar & Loretz GmbH	Cera de abelha, branca	191242004	1
Caesar & Loretz GmbH	Cera de abelha, branca	19124202	6
Caesar & Loretz GmbH	Cera de abelha, branca	19124203	5
Caesar & Loretz GmbH	Cera de abelha, branca	19124206	5
Caesar & Loretz GmbH	Cera de abelha, branca	19124210	4
Caesar & Loretz GmbH	Cera de abelha, branca	19124211	4
Caesar & Loretz GmbH	Cera de abelha, amarela	19137202	9
Caesar & Loretz GmbH	Cera de abelha, amarela	19137203	1
Caesar & Loretz GmbH	Cera de abelha, amarela	19137206	2
Caesar & Loretz GmbH	Palmitato de cetila	19139004	6
Caesar & Loretz GmbH	Palmitato de cetila	19139005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cera de abelha, amarela	19172001	1
Caesar & Loretz GmbH	Gordura sólida	191940001	3
Caesar & Loretz GmbH	Gordura sólida	191940002	11
Caesar & Loretz GmbH	Gordura sólida	19194001	1
Caesar & Loretz GmbH	Parafina sólida	192463001	8
Caesar & Loretz GmbH	Parafina sólida	192463010	2
Caesar & Loretz GmbH	Palmitato de cetila	192859002	4
Caesar & Loretz GmbH	Palmitato de cetila	192859003	18
Caesar & Loretz GmbH	Cera de abelha, amarela	20000280002	5
CAESAR & LORETZ GMBH	Cera de abelha, amarela	20000280003	1
Caesar & Loretz GmbH	Cera de abelha, amarela	20000280007	3
Caesar & Loretz GmbH	Cera de abelha, amarela	20000280008	5
Caesar & Loretz GmbH	Cera de abelha, branca	20000885003	6
Caesar & Loretz GmbH	Cera de abelha, branca	20000885004	2
Caesar & Loretz GmbH	Cera de abelha, branca	20000885007	13
Caesar & Loretz GmbH	Cera de abelha, branca	20000885008	1
Caesar & Loretz GmbH	Gordura sólida	20000906003	5
CAESAR & LORETZ GMBH	Gordura sólida	20000906003	2
Caesar & Loretz GmbH	Gordura sólida	20000906004	4
Caesar & Loretz GmbH	Gordura sólida	20000906005	2
Caesar & Loretz GmbH	Gordura sólida	20000906007	4
Caesar & Loretz GmbH	Gordura sólida	20000906008	2
Caesar & Loretz GmbH	Palmitato de cetila	20000974002	2
Caesar & Loretz GmbH	Palmitato de cetila	20000975002	5
Caesar & Loretz GmbH	Dodecilsulfato de sódio	20001260003	1
Caesar & Loretz GmbH	Manteiga de cacau	20001695002	2
Caesar & Loretz GmbH	Manteiga de cacau	20001695003	5
Caesar & Loretz GmbH	Cera de abelha, amarela	20001776002	2
Caesar & Loretz GmbH	Gordura sólida	20003131003	4
Caesar & Loretz GmbH	Gordura sólida	20003131004	2
Caesar & Loretz GmbH	Gordura sólida	20003131007	2
Caesar & Loretz GmbH	Gordura sólida	20003131008	5
Caesar & Loretz GmbH	Cera de abelha, amarela	20003602001	6
Caesar & Loretz GmbH	Cera de abelha, amarela	20003602002	4
Caesar & Loretz GmbH	Cera de abelha, amarela	20003602003	2
Caesar & Loretz GmbH	Cera de abelha, amarela	20003602005	6
Caesar & Loretz GmbH	Cera de abelha, amarela	20003602009	3
CAESAR & LORETZ GMBH	Cera de abelha, amarela	20003602009	1
Caesar & Loretz GmbH	Cera de abelha, branca	20003824003	2
Caesar & Loretz GmbH	Cera de abelha, amarela	20003825001	10
Caesar & Loretz GmbH	Palmitato de cetila	20003842006	1
Caesar & Loretz GmbH	Palmitato de cetila	20003842013	4
Caesar & Loretz GmbH	Manteiga de cacau	20004174002	2
Caesar & Loretz GmbH	Manteiga de cacau	20004174006	4
Caesar & Loretz GmbH	Manteiga de cacau	20004174010	2
Caesar & Loretz GmbH	Palmitato de cetila	21000359001	11
Caesar & Loretz GmbH	Parafina sólida	21000732001	10
Caesar & Loretz GmbH	Palmitato de cetila	21000860001	5
Caesar & Loretz GmbH	Palmitato de cetila	21000860009	3
Caesar & Loretz GmbH	Palmitato de cetila	21000860010	12
Caesar & Loretz GmbH	Cera de abelha, branca	21001267002	2
CAESAR & LORETZ GMBH	Cera de abelha, branca	21001267002	1
Caesar & Loretz GmbH	Cera de abelha, branca	21001267008	4
Caesar & Loretz GmbH	Cera de abelha, branca	21001267012	2
Caesar & Loretz GmbH	Cera de abelha, amarela	21001423001	2
Caesar & Loretz GmbH	Cera de abelha, amarela	21001423003	4
Caesar & Loretz GmbH	Cera de abelha, amarela	21001423004	5
Caesar & Loretz GmbH	Cera de abelha, amarela	21001423010	2
Caesar & Loretz GmbH	Parafina sólida	21001748004	5
Caesar & Loretz GmbH	Parafina sólida	21001748007	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Parafina sólida	21001748014	1
Caesar & Loretz GmbH	Manteiga de cacau	21002516002	3
Caesar & Loretz GmbH	Manteiga de cacau	21002516004	2
Caesar & Loretz GmbH	Manteiga de cacau	21002516017	1
Caesar & Loretz GmbH	Manteiga de cacau	21002516018	1
Caesar & Loretz GmbH	Manteiga de cacau	21002516020	2
Caesar & Loretz GmbH	Gordura sólida	21003046001	2
Caesar & Loretz GmbH	Gordura sólida	21003046008	14
Caesar & Loretz GmbH	Gordura sólida	21003046009	2
Caesar & Loretz GmbH	Gordura sólida	21003046011	5
Caesar & Loretz GmbH	Parafina, microcristalina	21003773003	1
Caesar & Loretz GmbH	Cera de abelha, amarela	21004132003	4
Caesar & Loretz GmbH	Palmitato de cetila	22000395002	3
Caesar & Loretz GmbH	Cera de abelha, branca	22000795006	2
Caesar & Loretz GmbH	Palmitato de cetila	22001717004	1
Caesar & Loretz GmbH	Gordura sólida	22002076002	1
Caesar & Loretz GmbH	Gordura sólida	22002076007	1
Caesar & Loretz GmbH	Gordura sólida	22002076010	3
Caesar & Loretz GmbH	Dodecilsulfato de sódio	22003127001	1
Caesar & Loretz GmbH	Cera de abelha, branca	2200795006	1
Caesar & Loretz GmbH	Dodecilsulfato de sódio	23000156006	1
Caesar & Loretz GmbH…	Palmitato de cetila	20000975002	1
Caesar & Loretz Hild…	Gordura sólida	20000906003	1
Caesar & Loretz Hild…	Cera de abelha, amarela	19137202	1
Caesar & Loretz/AHD	Cera de abelha, amarela	16038206	1
Caesar & Loretz/Gehe	Cera de abelha, amarela	191372001	1
Caesar & Loretz/Gehe	Cera de abelha, amarela	19137202	1
Caesar & Loretz/Geil…	Cera de abelha, amarela	19137202	2
Caesar & Loretz/Noweda	Cera de abelha, branca	191242001	1
Caesar & Loretz/Noweda	Cera de abelha, branca	19124210	1
Caesar & Loretz/Noweda	Parafina sólida	192463001	1
Caesar & Loretz/Noweda	Cera de abelha, branca	20000885004	1
Caesar & Loretz	Cera de abelha, amarela	15317613	1
Caesar & Loretz	Cera de abelha, amarela	16038201	1
Caesar & Loretz	Parafina sólida	18070107	1
Caesar / Ebert	Parafina sólida	15295405	1
Caesar / Gehe	Cera de abelha, amarela	15023004	1
Caesar / Gehe	Cera de abelha, amarela	15292009	1
Caesar Loretz Gmbh	Gordura sólida	17307602	1
Caesar u Loretz	Palmitato de cetila	14213710	1
Caesar und Loretz GmbH	Gordura sólida	18040401	1
Caesar&Lorenz	Cera de abelha, amarela	21001423001	1
Caesar&Loretz GmbH D…	Gordura sólida	11109617	1
Caesar&Loretz GmbH	Cera de abelha, amarela	16038210	1
Caesar&Loretz	Palmitato de cetila	17271504	2
Caesar/Gehe	Cera de abelha, branca	18048906	1
Caesar/Noweda	Cera de abelha, amarela	12124811	3
Caesar/Noweda	Palmitato de cetila	12228801	1
Caesar/Noweda	Cera de abelha, amarela	13031220	1
Caesar/Noweda	Palmitato de cetila	13295909	1
Caesar/Noweda	Gordura sólida	14126203	1
Caesar/Noweda	Palmitato de cetila	15301701	1
Caeser und Loretz GmbH	Gordura sólida	18333905	1
Caleo/ Noweda	Cera de abelha, amarela	18049003	1
Caleo/Sanacorp	Cera de abelha, amarela	18299201	1
calo	Cera de abelha, amarela	17011612	1
Carlo/Gehe/10,80	Palmitato de cetila	18273705	1
Carlo/Gehe/8,52	Cera de abelha, amarela	18299206	1
Cealo / Noweda	Manteiga de cacau	13292011	1
Cealo / Anzag	Parafina sólida	220826(21001748007)	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo/AHD	Parafina sólida	15295411	2
Cealo/Gehe	Cera de abelha, amarela	13335502	1
Cealo/GEHE	Palmitato de cetila	192859003	1
Cealo/Kehr	Cera de abelha, amarela	20000280002	1
Cealo/Noweda	Palmitato de cetila	22000395002	1
Cealo/Phoenix	Palmitato de cetila	20003842006	4
Cealo/Sanacorp	Gordura sólida	20003131007	1
Cealo	Cera de abelha, amarela	18113509	1
Cealo	Parafina sólida	21000732007	1
Cealo	Palmitato de cetila	21000860001	1
Ceasar & Loretz GmbH…	Palmitato de cetila	18149904	1
Cesar&Loretz GmbH Noweda	Palmitato de cetila	20000974002	1
China Medica	Gordura sólida	3244303	1
coelo/Sana	Palmitato de cetila	14351612	1
Cordes/Gehe	Cera de abelha, branca	18048907	1
E Plus	Cera de abelha, amarela	17011612	3
Ebert + Jacobi	Base para supositório (Wi…	20000603	3
E-Plus	Cera de abelha, amarela	16038202	1
Euro OTC	Cera de abelha, amarela	1201012-01	1
Euro OTC	Palmitato de cetila	12228808	1
Euro OTC	Parafina sólida	13109224	1
Euro OTC	Cera de abelha, amarela	1407013-01	1
Euro OTC	Manteiga de cacau	14123621	1
Euro OTC	Cera de abelha, amarela	1503013-01	1
Euro OTC	Gordura sólida	15185005	1
Euro OTC	Parafina sólida	15232004	1
Euro OTC	Palmitato de cetila	15301705	1
Euro OTC	Cera de abelha, amarela	16038201	1
Euro OTC	Palmitato de cetila	160419C	1
Euro OTC	Cera de abelha, branca	16163104	1
Euro OTC	Palmitato de cetila	16186809	1
Euro OTC	Manteiga de cacau	16316508	1
Euro OTC	Cera de abelha, amarela	17011607	1
Euro OTC	Cera de abelha, branca	17091802	1
Euro OTC	Gordura sólida	17107304	1
Euro OTC	Base para supositório (Wi…	17K09B03343780	1
Euro OTC	Gordura sólida	18004023	1
Euro OTC	Parafina sólida	18070107	1
Euro OTC	Cera de abelha, amarela	18113501	1
Euro OTC	Cera de abelha, amarela	18113505	3
Euro OTC	Palmitato de cetila	18149904	1
Euro OTC	Palmitato de cetila	19139005	2
Euro OTC	Palmitato de cetila	20000975002	1
Euro OTC	Palmitato de cetila	20003842013	1
Euro/Sanacorp	Cera de abelha, amarela	1708506	1
Euroo	Cera de abelha, amarela	1407013-01	1
Fagron	Gordura sólida		1
Fagron	Gordura sólida	12158115	2
Fagron	Palmitato de cetila	12C27-N07	2
Fagron	Palmitato de cetila	12D19-N02	1
Fagron	Cera de abelha, amarela	12D23-N05	2
Fagron	Gordura sólida	12G04-N18	1
Fagron	Gordura sólida	12I04-N11	1
Fagron	Gordura sólida	12K01-N12	1
Fagron	Gordura sólida	13243301	1
Fagron	Cera de abelha, amarela	13B04-N04	2
Fagron	Gordura sólida	13D10-N06	1
Fagron	Cera de abelha, amarela	13I02-B01	1
Fagron	Cera de abelha, amarela	13L02-B01-291452	1
Fagron	Cera de abelha, amarela	13L02-B01-294113	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cera de abelha, amarela	13L02-B01-294114	1
Fagron	Cera de abelha, amarela	14336616	1
Fagron	Gordura sólida	14G03-B03-296731	1
Fagron	Cera de abelha, amarela	14G07-B04-300495	3
Fagron	Gordura sólida	14L01-B06	2
Fagron	Gordura sólida	14L01-B06-303380	3
Fagron	Cera de abelha, branca	15292009	1
Fagron	Cera de abelha, branca	15292022	1
Fagron	Cera de abelha, amarela	15317603	1
Fagron	Base para supositório (Wi…	15A07-B12-309245	1
Fagron	Gordura sólida	15F03-B06	4
Fagron	Gordura sólida	15F03-B06-308708	3
Fagron	Base para supositório (Wi…	15J08-B04-322726	1
Fagron	Base para supositório (Wi…	15J08-B04-322727	1
Fagron	Base para supositório (Wi…	15J08-B04-324217	1
Fagron	Base para supositório (Wi…	15J08-B04-324959	2
Fagron	Dodecilsulfato de sódio	16229205	1
Fagron	Cera de abelha, branca	16a28_b10_322948	1
Fagron	Cera de abelha, branca	16A28-B10-322948	1
Fagron	Gordura sólida	16H01-B03-334976	2
Fagron	Cera de abelha, branca	16J28-B06	1
Fagron	Base para supositório (Wi…	16K08-B10-328956	1
Fagron	Base para supositório (Wi…	16K08-B10-332763	3
Fagron	Base para supositório (Wi…	16k08-b10-334910	1
Fagron	Base para supositório (Wi…	16K08-B10-339077	6
Fagron	Base para supositório (Wi…	16K09-B03-346709	1
Fagron	Base para supositório (Wi…	16K-B10-334910	1
Fagron	Cera de abelha, amarela	17011607	1
Fagron	Cera de abelha, branca	1701947	1
Fagron	Cera de abelha, branca	17091802	1
Fagron	Palmitato de cetila	17164005	1
Fagron	Parafina sólida	17245604	1
Fagron	Cera de abelha, branca	17C15-B01-342088	1
Fagron	Cera de abelha, branca	17C15-B01-354806	1
Fagron	Base para supositório (Wi…	17K09-B03	2
Fagron	Base para supositório (Wi…	17k09-b03-346709	1
Fagron	Base para supositório (Wi…	17K09-B03-346709	5
Fagron	Base para supositório (Wi…	17K09-B03-348770	4
Fagron	Base para supositório (Wi…	17k09-b03-351980	1
Fagron	Base para supositório (Wi…	17K09-B03-351980	5
Fagron	Base para supositório (Wi…	17K09-B03-355397	1
Fagron	Cera de abelha, branca	17L04-B05-348865	3
Fagron	Palmitato de cetila	18149904	1
Fagron	Dodecilsulfato de sódio	18182206	1
Fagron	Base para supositório (Wi…	18G13-B02	1
Fagron	Base para supositório (Wi…	18G13-B02-355398	1
Fagron	Base para supositório (Wi…	18G13-B02-356977	4
Fagron	Base para supositório (Wi…	18G13B02356978	1
Fagron	Gordura sólida	18I12-B04-354348	1
Fagron	Base para supositório (Wi…	19C04-B04	1
Fagron	Base para supositório (Wi…	19C04-B09	2
Fagron	Base para supositório (Wi…	19C04-B09-191420	2
Fagron	Base para supositório (Wi…	19C04B09191422	1
Fagron	Base para supositório (Wi…	19CO4-B04	1
Fagron	Gordura sólida	19I09-F04	2
Fagron	Gordura sólida	19I09-F04-365037	3
Fagron	Cera de abelha, branca	19J17-B01-196942	2
Fagron	Base para supositório (Wi…	20A08-B03	1
Fagron	Gordura sólida	20A08-B03-197663	2
Fagron	Base para supositório (Wi…	20A08-B03-197664	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Base para supositório (Wi…	20A08-B03-197665	1
Fagron	Palmitato de cetila	20B04-F08	1
Fagron	Gordura sólida	20B04-F08-368439	1
Fagron	Base para supositório (Wi…	20F10-B05	1
Fagron	Gordura sólida	20F10-B05-201350	2
Fagron	Base para supositório (Wi…	20G01-F02	1
Fagron	Gordura sólida	20G01-F02-372412	2
Fagron	Gordura sólida	20G01-F02-372412210030	1
Fagron	Gordura sólida	20G01-F02-376138	3
Fagron	Base para supositório (Wi…	20H17-B09-202675	3
Fagron	Base para supositório (Wi…	20J07-B02-202717	1
Fagron	Cera de abelha, branca	2155	1
Fagron	Base para supositório (Wi…	21D14-B12	1
Fagron	Base para supositório (Wi…	21D14-B12-216502	1
Fagron	Base para supositório (Wi…	21D14-B12-219382	1
Fagron	Base para supositório (Wi…	21D14-B12-219988	1
Fagron	Base para supositório (Wi…	22D12-B01	2
Fagron	Base para supositório (Wi…	22D12-B01-220445	1
Fagron	Base para supositório (Wi…	22D12-B01-224504	1
Fagron	Gordura sólida	22H04-B02-222151	2
Fagron	Base para supositório (Wi…	22J26-B12-229479	1
Fagron	Cera de abelha, amarela	280A140306	1
Fagron	Gordura sólida	20G01-F02-373358	1
Fagron	Base para supositório (Wi…	20J07-B02	1
Fagron	Base para supositório (Wi…	3518A-03934	1
Fagron	Base para supositório (Wi…	3914E-02328	1
Fagron	Base para supositório (Wi…	3917M-02328	1
Fagron	Gordura sólida	5628	1
Fagron	Gordura sólida	606469	1
Fagron	Base para supositório (Wi…	904381	1
Fagron	Gordura sólida	909394	2
Fagron	Base para supositório (Wi…	B02-2027107	1
Fagron	Base para supositório (Wi…	B0520134008	1
Fagron	Base para supositório (Wi…	B05-2013408	2
Fargon/Alliance HC	Palmitato de cetila	14351612	1
Fargon	Gordura sólida	20G01-F02-372412	2
Fargon	Gordura sólida	41319264	1
Fiebig	Gordura sólida	20000906003	1
Finze	Cera de abelha, amarela	10145002	1
Fischer/Phönix	Palmitato de cetila	15301711	1
Gatt-Koller	Manteiga de cacau	1803838	1
Gehe	Gordura sólida	11345918	1
Gehe	Cera de abelha, amarela	12079412	1
Gehe	Cera de abelha, amarela	12367910	1
Gehe	Gordura sólida	13243403	1
GEHE	Cera de abelha, amarela	13335502	1
Gehe	Dodecilsulfato de sódio	14127404	1
Gehe	Parafina sólida	14286511	1
Gehe	Cera de abelha, amarela	14336607	1
GEHE	Parafina sólida	15295409	1
Gehe	Parafina sólida	15295410	1
Gehe	Cera de abelha, amarela	16038207	1
GEHE	Cera de abelha, branca	16163109	1
GEHE	Dodecilsulfato de sódio	16229205	1
GEHE	Gordura sólida	16274203	1
Gehe	Parafina, microcristalina	17137508	1
Gehe	Cera de abelha, amarela	18049001	1
GEHE	Cera de abelha, amarela	18113501	1
GEHE	Gordura sólida	18147901	2
Gehe	Manteiga de cacau	19036008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Cera de abelha, branca	191242004	1
Gehe	Cera de abelha, branca	19124206	1
Gehe	Cera de abelha, amarela	19137202	1
Gehe	Gordura sólida	20003131008	1
Gehe	Parafina sólida	21001748007	1
Gehe	Cera de abelha, branca	22000795007	2
Gehe	Palmitato de cetila	22001785003	1
Gehe	Cera de abelha, amarela	22003888003	1
Gehe	Base para supositório (Wi…	22004876	1
Gehe	Dodecilsulfato de sódio	23000156007	2
gehe	Gordura sólida	23000561002	1
Gehe	Gordura sólida	23000561002	2
Gehe	Gordura sólida	23000561003	1
Gehe	Palmitato de cetila	8209646	1
Geibo	Cera de abelha, amarela	290A170915	1
Gutenberg-Apotheke	Manteiga de cacau	13292007	1
Hänseler	Cera de abelha, amarela		6
HCK	Parafina sólida	16277705	1
Hedinger GmbH/Noweda	Parafina sólida	17347701	1
Henry Lamotte/ Allia…	Manteiga de cacau	19036003	1
Hirsch	Cera de abelha, amarela	12257012	1
Ichthyol/Phönix	Dodecilsulfato de sódio	15344510	1
Ichthyol	Cera de abelha, amarela	13031239	1
Intern Drogen	Dodecilsulfato de sódio	216991080	1
INTERN-DROGEN	Gordura sólida	20003131003	1
INTERN-DROGEN	Cera de abelha, branca	20003825001	2
INTERN-DROGEN	Cera de abelha, amarela	21001423005	1
INTERN-DROGEN	Parafina sólida	21001748004	3
Jenne	Parafina sólida	17347701	1
Jenne	Cera de abelha, branca	22003630003	2
Jenne	Palmitato de cetila	23001428006	1
Jenne	Cera de abelha, branca	23002638001	1
Kehr	Parafina sólida	17347701	1
Kehr	Base para supositório (Wi…	17K09-B03-351980	1
Kehr	Cera de abelha, branca	18048906	1
Kehr	Cera de abelha, amarela	18113501	1
Kehr	Cera de abelha, branca	21001267012	1
Kehr	Cera de abelha, amarela	21004132003	2
Kehr	Cera de abelha, branca	22003630003	2
Klenk	Cera de abelha, branca	10503-01	1
Klenk	Cera de abelha, amarela	13335513	1
Klenk	Cera de abelha, amarela	160311	1
Klenk	Cera de abelha, branca	19071005	1
Klenk	Cera de abelha, amarela	190A170314	1
Klenk	Cera de abelha, amarela	20110-01	1
Klenk	Cera de abelha, amarela	20110-03	1
Klenk	Cera de abelha, branca	20609-01	2
Klenk	Cera de abelha, amarela	220110-002	1
Klenk	Cera de abelha, branca	221115-001	1
Klenk	Cera de abelha, branca	230413-001	1
Klenk	Cera de abelha, amarela	280A110110	1
Klenk	Cera de abelha, amarela	280A120627	5
Klenk	Cera de abelha, amarela	280-A120627	1
Klenk	Cera de abelha, amarela	280A130115	26
Klenk	Cera de abelha, amarela	280A13011A	1
Klenk	Cera de abelha, amarela	280A140306	7
Klenk	Cera de abelha, amarela	280A150528	13
Klenk	Cera de abelha, branca	280A160311	17
Klenk	Cera de abelha, amarela	280A171019	31
Klenk	Cera de abelha, branca	280A190715	18

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Cera de abelha, branca	280A190715-01	1
Klenk	Cera de abelha, branca	280A2008005-01	1
Klenk	Cera de abelha, branca	280A200804	1
Klenk	Cera de abelha, branca	280A200804-01	6
Klenk	Cera de abelha, branca	280A200805-01	3
Klenk	Cera de abelha, branca	280A210503-01	9
Klenk	Cera de abelha, branca	280A220609-01	1
Klenk	Cera de abelha, branca	280A220609-02	2
Klenk	Cera de abelha, branca	280A221115-01	2
Klenk	Cera de abelha, amarela	282A120627	1
Klenk	Cera de abelha, amarela	282A140306	1
Klenk	Cera de abelha, amarela	290A081210	1
Klenk	Cera de abelha, amarela	290A110803	1
Klenk	Cera de abelha, amarela	290A120627	4
Klenk	Cera de abelha, amarela	290A140903	5
Klenk	Cera de abelha, amarela	290A150716	5
Klenk	Cera de abelha, amarela	290A151214	5
Klenk	Cera de abelha, amarela	290A170314	5
Klenk	Cera de abelha, amarela	290A170915	15
Klenk	Cera de abelha, amarela	290A200108-01	1
Klenk	Cera de abelha, amarela	290A200108-02	2
Klenk	Cera de abelha, amarela	290A220110-002	1
Klenk	Cera de abelha, amarela	290A220110-01	3
Klenk	Cera de abelha, amarela	290A220110-02	2
Klenk	Cera de abelha, amarela	290A230120-01	1
Klenk	Cera de abelha, amarela	290A230413-01	1
Klenk	Cera de abelha, amarela	416E01240	1
Klenk	Cera de abelha, branca	804-01	1
Klenk	Cera de abelha, branca	805-01	1
Krieger	Gordura sólida	23000447	1
L10	Palmitato de cetila	16053811	1
L10	Palmitato de cetila	16186805	1
L10	Cera de abelha, amarela	17207403	1
L12	Manteiga de cacau	16316508	1
L12	Parafina, microcristalina	17137502	1
L12	Cera de abelha, amarela	18113502	1
L12	Cera de abelha, amarela	18113506	1
L12	Palmitato de cetila	18149904	2
L30	Palmitato de cetila	17271505	1
L30	Parafina sólida	17347701	1
Lamotte/Allia	Gordura sólida	18004024	1
Mittelwand bio 2017	Cera de abelha, amarela	5022017	1
Nachprüfung vom 31.0…	Gordura sólida	15185002	1
Nachprüfung	Palmitato de cetila	123456	1
Nachprüfung	Parafina sólida	18070131	1
Nachprüfung	Palmitato de cetila	3012U01241	1
Nachprüfung	Palmitato de cetila	4917I-01242	1
Noweda	Manteiga de cacau	11117813	2
Noweda	Gordura sólida	11345909	1
Noweda	Parafina sólida	11363206	1
Noweda	Cera de abelha, amarela	12124810	1
Noweda	Parafina, microcristalina	12266304	1
Noweda	Parafina sólida	14286517	1
Noweda	Cera de abelha, amarela	150230004	1
Noweda	Cera de abelha, amarela	15023002	1
Noweda	Base para supositório (Wi…	16027801	1
Noweda	Cera de abelha, branca	16163114	1
Noweda	Parafina sólida	16277710	1
Noweda	Parafina sólida	163277710	1
Noweda	Palmitato de cetila	17271505	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Parafina sólida	17347701	1
Noweda	Base para supositório (Wi…	18006248	1
Noweda	Cera de abelha, branca	18048901	1
noweda	Cera de abelha, amarela	18049001	1
Noweda	Gordura sólida	18147901	1
Noweda	Cera de abelha, branca	18239106	1
Noweda	Gordura sólida	18333904	1
Noweda	Palmitato de cetila	19139004	1
Noweda	Cera de abelha, amarela	20000280008	2
Noweda	Cera de abelha, branca	20000885007	1
Noweda	Cera de abelha, branca	21001267002	3
Noweda	Cera de abelha, amarela	21001423001	2
Noweda	Cera de abelha, amarela	21001423003	1
Noweda	Cera de abelha, amarela	21001423005	1
Noweda	Parafina sólida	21001748004	2
Noweda	Parafina sólida	2100174801	1
Noweda	Parafina sólida	21001748012	2
Noweda	Cera de abelha, branca	22000795001	1
Noweda	Gordura sólida	23000561002	1
Noweda	Cera de abelha, amarela	280A120627	2
Noweda	Cera de abelha, amarela	290A23012001	1
Noweda	Cera de abelha, amarela	290A230120-01	1
Noweda	Cera de abelha, amarela	290A230413-01	1
Otto	Cera de abelha, amarela	WG10052021	1
Ph.Eur.	Cera de abelha, amarela	17207402	1
Pharmachem	Cera de abelha, branca	15292014	1
Pharmachem	Cera de abelha, amarela	16038202	1
PHOENIX 24.07.2014	Cera de abelha, amarela	13001206	1
Phoenix 3.3.14	Gordura sólida	13243414	1
Phoenix goettingen 08.05	Cera de abelha, amarela	15098901	1
Phoenix goettingen 09.05	Parafina sólida	13390415	1
Phoenix	Palmitato de cetila	14060705	1
Phoenix	Cera de abelha, branca	15292003	1
Phoenix	Parafina sólida	15295410	1
Phoenix	Cera de abelha, branca	16163109	1
Phoenix	Base para supositório (Wi…	16k08-b10-332763	1
Phoenix	Palmitato de cetila	17164005	1
Phoenix	Parafina sólida	18070131	1
Phoenix	Palmitato de cetila	18149912	1
Phoenix	Gordura sólida	18333904	1
Phoenix	Cera de abelha, branca	19124206	1
Phoenix	Cera de abelha, amarela	20000280008	1
Phoenix	Parafina sólida	21000732007	1
Phoenix	Cera de abelha, branca	21001267002	1
Phoenix	Gordura sólida	21003046011	2
Phoenix	Palmitato de cetila	22001717001	1
Phoenix	Dodecilsulfato de sódio	23000156006	1
Phoenix	Cera de abelha, branca	280A221115-01	1
Phoenix	Base para supositório (Wi…	3076	1
Phönix / 2	Cera de abelha, amarela	20000280002	1
Phönix, Caesar&Loret…	Cera de abelha, amarela	191372001	1
Phönix	Cera de abelha, amarela	10849001	1
Phönix	Cera de abelha, amarela	12367901	1
Phönix	Cera de abelha, amarela	12367904	1
Phönix	Cera de abelha, amarela	12367915	1
Phönix	Cera de abelha, amarela	13031206	1
Phönix	Palmitato de cetila	13131906	1
Phönix	Parafina, microcristalina	13274301	1
Phönix	Palmitato de cetila	13295919	1
phönix	Cera de abelha, branca	15292022	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Palmitato de cetila	15301711	1
Phönix	Cera de abelha, amarela	15317609	1
Phönix	Cera de abelha, amarela	16038206	2
phönix	Cera de abelha, amarela	16038207	1
phönix	Cera de abelha, branca	16163109	1
Phönix	Gordura sólida	16274203	1
PHÖNIX	Cera de abelha, amarela	17011611	1
Phönix	Palmitato de cetila	17043504	1
Phönix	Manteiga de cacau	17314902	1
Phönix	Gordura sólida	18000346	1
Phönix	Cera de abelha, amarela	18049001	1
Phönix	Cera de abelha, amarela	18113501	1
Phönix	Manteiga de cacau	18135106	1
Phönix	Gordura sólida	18147902	2
Phönix	Palmitato de cetila	18149912	1
Phönix	Manteiga de cacau	19000676003	4
Phönix	Manteiga de cacau	19036011	3
Phönix	Palmitato de cetila	19139004	1
Phönix	Parafina sólida	192463010	1
Phönix	Palmitato de cetila	192869002	1
Phönix	Manteiga de cacau	2000169002	1
Phönix	Cera de abelha, amarela	20003602005	1
Phönix	Cera de abelha, branca	20003825001	1
Phönix	Parafina sólida	21000732007	1
Phönix	Cera de abelha, amarela	21001423003	3
Phönix	Palmitato de cetila	22001717004	1
Phönix	Manteiga de cacau	27121	1
Phönix	Gordura sólida	277212	1
Phönix	Cera de abelha, branca	280A171019	1
Phönix	Base para supositório (Wi…	B05-2013409	1
Phytocomm	Gordura sólida	209314	1
Purren Apotheke	Gordura sólida	10I03-N08	1
Rondell Apotheke	Gordura sólida	15185002	1
Sanacorp 03.01.22	Palmitato de cetila	220103CP	1
Sanacorp WE:18.04.16…	Cera de abelha, amarela	15023004	1
Sanacorp	Cera de abelha, amarela		1
Sanacorp	Manteiga de cacau	1121300203	1
Sanacorp	Cera de abelha, amarela	12257009	1
Sanacorp	Cera de abelha, amarela	12367910	1
Sanacorp	Manteiga de cacau	13027207	1
sanacorp	Manteiga de cacau	13140407	1
Sanacorp	Cera de abelha, amarela	13335502	1
Sanacorp	Cera de abelha, amarela	13378619	1
Sanacorp	Gordura sólida	14126203	1
sanacorp	Gordura sólida	14338703	1
Sanacorp	Cera de abelha, amarela	16038203	1
Sanacorp	Cera de abelha, branca	16163105	1
Sanacorp	Cera de abelha, branca	16163114	1
Sanacorp	Palmitato de cetila	16186805	1
Sanacorp	Gordura sólida	16274202	1
Sanacorp	Cera de abelha, amarela	17011604	2
Sanacorp	Cera de abelha, amarela	17011609	1
Sanacorp	Cera de abelha, amarela	17011612	1
Sanacorp	Palmitato de cetila	17043504	1
Sanacorp	Manteiga de cacau	17055908	3
Sanacorp	Manteiga de cacau	170559908	1
Sanacorp	Palmitato de cetila	17164004	1
Sanacorp	Manteiga de cacau	17314902	1
Sanacorp	Base para supositório (Wi…	17k09-b03-346709	1
Sanacorp	Parafina sólida	18070131	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Cera de abelha, amarela	18113501	1
Sanacorp	Cera de abelha, amarela	18113502	1
Sanacorp	Manteiga de cacau	18135106	3
Sanacorp	Gordura sólida	18147907	1
Sanacorp	Cera de abelha, branca	18239106	1
Sanacorp	Cera de abelha, amarela	18299201	1
Sanacorp	Cera de abelha, branca	191242002	1
Sanacorp	Cera de abelha, amarela	191372001	1
Sanacorp	Cera de abelha, amarela	19137202	1
Sanacorp	Parafina sólida	19246300	1
Sanacorp	Palmitato de cetila	192859003	1
Sanacorp	Palmitato de cetila	192859005	1
Sanacorp	Cera de abelha, amarela	20000280008	1
Sanacorp	Palmitato de cetila	20000975002	1
Sanacorp	Cera de abelha, branca	20003825001	1
Sanacorp	Cera de abelha, amarela	21001423001	1
Sanacorp	Cera de abelha, amarela	21004132003	1
Sanacorp	Palmitato de cetila	22000395002	1
Sanacorp	Cera de abelha, branca	22000795001	1
Sanacorp	Palmitato de cetila	22001717004	2
Sanacorp	Cera de abelha, branca	22003630003	2
Sanacorp	Cera de abelha, amarela	22003888003	1
Sanacorp	Gordura sólida	23000561002	3
Sanacorp	Cera de abelha, branca	280A171019	1
Sanacorp	Cera de abelha, amarela	290A230413-01	2
Sanacorp	Dodecilsulfato de sódio	5/AKD1	1
Sanacorp	Dodecilsulfato de sódio	5/AKD6	1
Sanacorp	Palmitato de cetila	8/AKD12	1
Sanacorp	Palmitato de cetila	8/AKD13	1
Sanacorp	Manteiga de cacau	AKD27	1
Sanacorp	Manteiga de cacau	AKD28	1
Spinnrad / Phönix	Manteiga de cacau	719300202	1
Spinnrad/ Noweda/ 08…	Manteiga de cacau	920300201	1
Spinnrad/ Sanacorp 2…	Manteiga de cacau	719300202	1
Spinnrad/GEHE	Manteiga de cacau	920300201	1
Spinnrad/Noweda	Cera de abelha, branca	118048061	2
Spinnrad/Noweda	Manteiga de cacau	317300201	1
Spinnrad/Noweda	Manteiga de cacau	717300202	1
Spinnrad	Manteiga de cacau	1017300203	1
Spinnrad	Manteiga de cacau	1017300212	1
Spinnrad	Cera de abelha, branca	1018048062	1
Spinnrad	Cera de abelha, branca	1121402003	1
Spinnrad	Cera de abelha, branca	118048061	1
spinnrad	Manteiga de cacau	1218300203	1
Spinnrad	Manteiga de cacau	221302051	1
Spinnrad	Cera de abelha, branca	317048061	1
Spinnrad	Manteiga de cacau	319300201	1
spinnrad	Manteiga de cacau	3252	1
Spinnrad	Manteiga de cacau	512300202	1
spinnrad	Cera de abelha, branca	718402002	1
Symbiotica	Palmitato de cetila	2208030-01	1
Unisan	Parafina sólida	11166911	3
Wachs neu	Cera de abelha, amarela		2

- 230 341 spectra from 1515 *Apo-Ident* customers from a total of 48 157 batches from a further 713 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ceras/gorduras* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ceras/gorduras* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	2847	0	150 115
Type B	0	2198	5	199 881
Type C	0	5721	5	230 341

The substance/substance group *Ceras/gorduras* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.7893 %)
Type B	100.0000 % (> 99.9912 %)	99.7730 % (> 99.6369 %)
Type C	100.0000 % (> 99.9007 %)	99.9127 % (> 99.8603 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20865	20865	0,00	151,88
20986	20986	0,00	109,73
21067	22479	14,26	147,84
21433	23511	5,33	135,55
21482	24813	16,93	150,07
21483	21483	0,00	88,86
21682	21682	0,00	67,37
21731	22349	2,94	126,00
21766	22330	6,77	70,31
21875	23639	5,52	128,58
21880	21880	0,00	139,00
21984	21984	0,00	142,69
22244	23511	8,74	139,86
22245	23511	5,69	126,81
22325	21984	4,16	124,78
22330	22330	0,00	68,28

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22338	21880	5,97	138,52
22348	23067	7,52	142,80
22349	22349	0,00	129,49
22352	23278	13,73	102,80
22479	22479	0,00	142,34
22486	22486	0,00	113,40
22956	23511	19,71	137,96
23067	23067	0,00	146,24
23242	24715	12,53	102,45
23278	23278	0,00	98,05
23511	23511	0,00	131,08
23560	23817	7,32	127,85
23565	23067	44,60	146,04
23601	21880	5,59	139,15
23639	23639	0,00	122,66
23705	23067	45,23	147,01
23707	23067	6,57	146,32
23817	23817	0,00	111,94
24715	24715	0,00	95,22
24716	24716	0,00	96,68
24720	24720	0,00	138,15
24813	24813	0,00	148,94
24870	23511	4,42	135,82
25047	21880	13,55	140,32
25216	25216	0,00	93,48
25381	22479	23,83	146,37
25384	23067	6,02	153,74
25387	22349	7,54	144,35
25434	27418	14,29	138,17
25445	21880	9,03	140,46
25639	25639	0,00	142,58
25723	25723	0,00	76,72
25739	23511	18,08	106,37
26108	26108	0,00	94,37
26362	26362	0,00	140,62
26622	23511	38,42	159,61
26696	26696	0,00	95,62
26734	25723	19,04	101,51
26745	22349	6,38	128,80
26910	23511	8,25	114,97
26959	26959	0,00	112,86
27034	21880	17,15	141,39
27268	23511	19,72	106,98
27418	27418	0,00	144,55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cetoconazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20688-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cetoconazol

Special notes

When selecting the *Cetoconazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cetoconazol	6	3	77

Second-stage model

For differentiation of the substance/substance group *Cetoconazol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cetoconazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	116,96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cetoconazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cetoconazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cetoconazol	12171007	20688	30	1401554
Caelo	Cetoconazol	13179612	21514	60	20130613
Caelo	Cetoconazol	13179612	21515	60	20130613
Caelo	Cetoconazol	153477	24028	40	20151113*
Fagron	Cetoconazol	12A16-N06	20699	40	20120123
Fagron	Cetoconazol	16A26-B01-322982	23183	40	20160210
Fagron	Cetoconazol	20H18-F03-375993	25666	50	20201116

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Cetoconazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Cetoconazol*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cetoconazol	20002966003	25430	40
Fagron	Cetoconazol	17H14-B01-339422	23917	40
Fagron	Cetoconazol	21K18-B06-213329	26281	40
Fagron	Cetoconazol	20H18-F03-375993	25666SI†	10
Fagron	Cetoconazol	21K18-B06-213329	26281SI	20

- 201 934 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 258 spectra from 145 *Apo-Ident* customers from 80 batches from the substance/substance group *Cetoconazol*.

- Among them are spectra of independent samples from 77 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cetoconazol	20003758006	1
	Cetoconazol	20003758009	2
	Cetoconazol	20003758017	1
	Cetoconazol	21k18-b06	1
Alliance Healthcare	Cetoconazol	20002966003	1
ANZAG 23.07.14	Cetoconazol	13h09-n07	1
Caelo	Cetoconazol	11070001	1
Caelo	Cetoconazol	11070022	1
Caelo	Cetoconazol	12300406	1
Caelo	Cetoconazol	12300407	2
Caelo	Cetoconazol	13179601	2
Caelo	Cetoconazol	13179606	3
Caelo	Cetoconazol	13179612	2
Caelo	Cetoconazol	13399404	8
Caelo	Cetoconazol	13399408	7
Caelo	Cetoconazol	13399412	3
Caelo	Cetoconazol	14350408	4
Caelo	Cetoconazol	14350416	4
Caelo	Cetoconazol	14350419	1
Caelo	Cetoconazol	14350420	2
Caelo	Cetoconazol	14350421	1
Caelo	Cetoconazol	14350422	3
Caelo	Cetoconazol	14350427	2
Caelo	Cetoconazol	14350429	6
Caelo	Cetoconazol	14350434	2
Caelo	Cetoconazol	14350436	3
Caelo	Cetoconazol	14350437	7
Caelo	Cetoconazol	14350442	3
Caelo	Cetoconazol	14k04-b06-309671	1
Caelo	Cetoconazol	15347701	13
Caelo	Cetoconazol	18007003	6
Caelo	Cetoconazol	18007004	2
Caelo	Cetoconazol	18007011	5
Caelo	Cetoconazol	18007013	2
Caelo	Cetoconazol	18007015	9
Caelo	Cetoconazol	18007016	1
Caelo	Cetoconazol	18007020	2
Caelo	Cetoconazol	1906611	1
Caelo	Cetoconazol	19096601	6
Caelo	Cetoconazol	19096605	2
Caelo	Cetoconazol	19096609	1
Caelo	Cetoconazol	19096611	4
Caelo	Cetoconazol	20002966001	1
Caelo	Cetoconazol	20002966002	2
Caelo	Cetoconazol	20002966003	9
Caelo	Cetoconazol	20003758004	4
Caelo	Cetoconazol	20003758005	6
Caelo	Cetoconazol	20003758006	2
Caelo	Cetoconazol	20003758009	1
Caelo	Cetoconazol	2003758005	1
Caelo	Cetoconazol	53317046	2
Caeolo /Gehe	Cetoconazol	14350408	1
Caesar & Loretz GmbH...	Cetoconazol	19096601	1
Caesar & Loretz GmbH/AHD	Cetoconazol	19096611	1
Caesar & Loretz GmbH/AHD	Cetoconazol	20003758005	1
Caesar & Loretz GmbH...	Cetoconazol	19096601	1
Caesar & Loretz GmbH...	Cetoconazol	19096611	1
Caesar & Loretz GmbH/Gehe	Cetoconazol	20003758005	1
Caesar & Loretz GmbH...	Cetoconazol	20002966003	2
Caesar & Loretz GmbH...	Cetoconazol	20002966003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH…	Cetoconazol	20003758004	2
Caesar & Loretz GmbH	Cetoconazol	18007015	2
Caesar & Loretz GmbH	Cetoconazol	19096601	1
Caesar & Loretz GmbH	Cetoconazol	19096608	1
Caesar & Loretz GmbH	Cetoconazol	19096611	2
Caesar & Loretz GmbH	Cetoconazol	20002966002	1
Caesar & Loretz GmbH	Cetoconazol	20002966003	9
Caesar & Loretz GmbH	Cetoconazol	20003758004	4
Caesar & Loretz GmbH	Cetoconazol	20003758005	4
Caesar & Loretz GmbH	Cetoconazol	20003758006	3
Caesar & Loretz/AHD	Cetoconazol	18007015	1
E Plus	Cetoconazol	14350429	1
Euro OTC	Cetoconazol	13179615	1
Fagron	Cetoconazol	12I17-N02	1
Fagron	Cetoconazol	13179613	1
Fagron	Cetoconazol	13H09-N07	1
Fagron	Cetoconazol	13J23-N04	1
Fagron	Cetoconazol	14E09-B01-293736	3
Fagron	Cetoconazol	14E09-B01-297637	2
Fagron	Cetoconazol	14K04-B06-309671	3
Fagron	Cetoconazol	15G23-B03-312063	1
Fagron	Cetoconazol	15G23-B03-316596	2
Fagron	Cetoconazol	16A26-B01-327490	1
Fagron	Cetoconazol	16A26-B01-335467	3
Fagron	Cetoconazol	17H14-B01-339006	1
Fagron	Cetoconazol	17H14-B01-339422	1
Fagron	Cetoconazol	17H14-B01-344222	2
Fagron	Cetoconazol	17H14-B01-353376	1
Fagron	Cetoconazol	17h14-b01-353378	1
Fagron	Cetoconazol	17H14-B01-353378	1
Fagron	Cetoconazol	18E28-B02-359205	2
Fagron	Cetoconazol	18E28-B02-364169	4
Fagron	Cetoconazol	20h18-F03-375071	1
Fagron	Cetoconazol	20H18-F03-375071	2
Fagron	Cetoconazol	20H18-F03-375073	1
Fagron	Cetoconazol	21k18-bo6	1
Fagron	Cetoconazol	5015E-02866	1
Fagron	Cetoconazol	700669-0001	1
Fagron	Cetoconazol	KET/11707237	1
Fagron	Cetoconazol	KET/12007311	1
Fiebig	Cetoconazol	14350437	1
Fiebig	Cetoconazol	19096601	1
Gehe	Cetoconazol	11070019	1
Gehe	Cetoconazol	14350427	1
Gehe	Cetoconazol	20003758006	2
Gehe	Cetoconazol	20003758009	1
Noweda	Cetoconazol	19096601	1
Phoenix	Cetoconazol	19096601	1
Phönix/Caesar&Lorenz…	Cetoconazol	20003758005	1
Phönix	Cetoconazol	12171018	1
Phönix	Cetoconazol	18007003	1
Sanacorp Stralsund	Cetoconazol	20003758005	1
Sanacorp	Cetoconazol	13179602	3
Sanacorp	Cetoconazol	20003758006	1

- 235 809 spectra from 1515 *Apo-Ident* customers from a total of 49 178 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cetoconazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cetoconazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	150	0	201 934
Type C	0	255	3	235 809

The substance/substance group *Cetoconazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.8372 % (> 97.6744 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20688	20688	0,00	205,65
20699	24028	12,27	210,53
21514	24028	10,45	210,41
21515	24028	19,37	206,13
23183	24028	18,30	210,36
24028	24028	0,00	212,29
25666	24028	30,64	202,29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cianocobalamina/Metilcobalamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10003566-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cianocobalamina/Metilcobalamina; Cianocobalamina; Cyanocobalaminum; Metilcobalamina

Special notes

When selecting the *Cianocobalamina/Metilcobalamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cianocobalamina/Metilcobalamina	16	10	33

Second-stage model

For differentiation of the substance/substance group *Cianocobalamina/Metilcobalamina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cianocobalamina/Metilcobalamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Bacitracina	40,78	14,86
Sulfato de polimixina B	45,31	24,47
⋮	⋮	⋮
Sulfato de colistina	>50	29,63
Anfotericina B	>50	30,21
Pantotenato de cálcio	>50	43,53
Nistatina	>50	47,58
Estriol	>50	55,16
Gelatina, branca	>50	55,44
Triancinolona	>50	59,83
Vitamina E acetato pó 50%	>50	72,47
Estradiol hemi-hidratado	>50	74,06
Riboflavina	>50	81,64
Bromidrato de hioscina	>50	104,50
Glicerofosfato de cálcio	>50	120,60
Tosilcloramida sódica	>50	128,79
Levedura de selênio	>50	140,93
Carmelose sódica	>50	158,58
SyrSpend® SF Alka	>50	161,50
SyrSpend® SF pH4 neo	>50	176,13
Ácido oxálico	>50	189,49
Amido de arroz	>50	194,41
SyrSpend® SF pH4	>50	244,54
Amido de milho	>50	272,47
Goma arábica, dispersão seca	>50	286,28
Amido de trigo	>50	361,94
Fécula de batata	>50	368,81
Maltodextrina	>50	389,50
Frutose	>50	415,02

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cianocobalamina/Metilcobalamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cianocobalamina/Metilcobalamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cianocobalamina	13342803	21299	40	AR-15-FG-005429-01
Caelo	Cianocobalamina	13342807	21479	60	AR-15-FG-014917-01
Caelo	Cianocobalamina	13342807	21479SI	30	AR-15-FG-014917-01
Caelo	Cianocobalamina	160154	22441	60	20160309*
Caelo	Cianocobalamina	160154	22441SI	60	20160309*
Euro OTC	Cianocobalamina	1305040-01	21635	60	AR-15-FG-005214-01
Euro OTC	Cianocobalamina	1506035	21867	60	20150708*
Euro OTC	Cianocobalamina	1506035	21867SI	60	20150708*
Euro OTC	Cianocobalamina	1506035	21872	60	0000010479
Euro OTC	Cianocobalamina	1506035	21872SI	45	0000010479
Euro OTC	Cianocobalamina	1604017	22536	30	20160509*
Euro OTC	Cianocobalamina	1604017	22536SI	30	20160509*
Euro OTC	Cianocobalamina	1812011	24465	40	20190205*
Euro OTC	Metilcobalamina	1207019-01	20743	40	1402501
Euro OTC	Metilcobalamina	1401032-01	21721	60	8778
Euro OTC	Metilcobalamina	1510002	22234	60	20151201*
Euro OTC	Metilcobalamina	1401032	22239	60	20151201*
Euro OTC	Metilcobalamina	1601043	22379	60	20160209*
Euro OTC	Metilcobalamina	1804006	24072	40	20180420*
Euro OTC	Metilcobalamina	1809001	24311	40	20180925*
Euro OTC	Metilcobalamina	1904002	24775	40	20190806*
Euro OTC	Metilcobalamina	2002014	25135	40	20200401*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1075 spectra of 22 reference samples from the substance/substance group *Cianocobalamina/Metilcobalamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 16 different batches.
- 151 887 spectra from a total of 2826 batches from further 484 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 680 spectra of 18 reference samples from the substance/substance group *Cianocobalamina/Metilcobalamina*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cianocobalamina	16015411	23761	40
Caelo	Cianocobalamina	162215	23790	40
Caelo	Cianocobalamina	21001468003	25976	40
Euro OTC	Cianocobalamina	1907030	24965	40
Euro OTC	Cianocobalamina	2109009	25868	50
Euro OTC	Cianocobalamina	2206015	26272	40
Fagron	Cianocobalamina	23H14-B07-230965	27022	40
Euro OTC	Metilcobalamina	1711031	23885	40
Euro OTC	Metilcobalamina	2006003	25412	40
Euro OTC	Metilcobalamina	2202009	26097	40
Caelo	Cianocobalamina	13342807	21479SI†	30
Caelo	Cianocobalamina	21001468003	25976SI	40
Euro OTC	Cianocobalamina	1604017	22536SI†	10
Euro OTC	Cianocobalamina	1907030	24965SI	40
Euro OTC	Cianocobalamina	2109009	25868SI	50
Euro OTC	Cianocobalamina	2206015	26272SI	40
Fagron	Cianocobalamina	23H14-B07-230965	27022SI	40
Euro OTC	Metilcobalamina	2202009	26097SI	20

- 201 404 spectra from a total of 4033 batches from further 841 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 39 spectra from 25 *Apo-Ident* customers from 33 batches from the substance/substance group *Cianocobalamina/Metilcobalamina*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cianocobalamina	19I20-B04-1955509	1
	Cianocobalamina	20D06-B02-2016102	1
Caelo	Cianocobalamina	16015405	1
Caelo	Cianocobalamina	1604017-01	1
Caelo	Cianocobalamina	18016001	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cianocobalamina	18016010	1
Caelo	Cianocobalamina	19088601	1
Caelo	Cianocobalamina	19I20-B04	1
Caelo	Cianocobalamina	21001468003	1
Caelo	Cianocobalamina	21001468005	1
Caelo	Cianocobalamina	9324102	1
Caelo	Cianocobalamina	9324113	1
Caelo	Cianocobalamina	9351704	1
Caelo	Cianocobalamina	9373503	2
Caesar & Loretz GmbH…	Cianocobalamina	9324102	1
Caesar & Loretz GmbH	Cianocobalamina	16221501	1
EuRho	Cianocobalamina	1812011-01	1
Euro OTC	Metilcobalamina	1601043-02	1
Euro OTC	Metilcobalamina	1711031-01	1
Euro OTC	Metilcobalamina	1804006-01	1
Euro OTC	Metilcobalamina	1809001-01	1
Euro OTC	Metilcobalamina	2002014-01	1
Euro OTC	Metilcobalamina	2006003-01	3
Euro OTC	Metilcobalamina	2006003-02	1
Euro OTC	Cianocobalamina	5061204	1
Fagron	Cianocobalamina	10K02-N05	2
Fagron	Cianocobalamina	10K02-NO5	1
Fagron	Cianocobalamina	13124-B01-292062	1
Fagron	Cianocobalamina	15H31-B02-315113	1
Fagron	Cianocobalamina	17A27-B04	1
Fagron	Cianocobalamina	17A27-B04-339672	2
Fagron	Cianocobalamina	B04-3396702	1
faron	Cianocobalamina	18/10-B01-357181	1
Spinnrad/Phoenix	Cianocobalamina	1217331032	1

- 236 028 spectra from 1515 *Apo-Ident* customers from a total of 49 225 batches from a further 720 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cianocobalamina/Metilcobalamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cianocobalamina/Metilcobalamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1075	0	151 887
Type B	0	680	0	201 404
Type C	0	38	1	236 028

The substance/substance group *Cianocobalamina/Metilcobalamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4419 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1176 %)
Type C	100.0000 % (> 99.9007 %)	97.4359 % (> 89.7436 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20743	20743	0,00	71,31
21299	21299	0,00	52,30
21479	21479	0,00	57,69
21635	21635	0,00	45,10
21721	21721	0,00	107,55
21867	21867	0,00	46,96
21872	21872	0,00	61,16
22234	22234	0,00	40,78
22239	22239	0,00	67,66
22379	22379	0,00	55,94
22441	22441	0,00	96,37
22536	22536	0,00	88,83
24072	24072	0,00	52,17
24311	24311	0,00	60,77
24465	24465	0,00	74,85
24775	24775	0,00	73,32
25135	25135	0,00	101,46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ciclamato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20917-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ciclamato de sódio; Natrii cyclamas

Special notes

When selecting the *Ciclamato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ciclamato de sódio	6	3	40

Second-stage model

For differentiation of the substance/substance group *Ciclamato de sódio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ciclamato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	114,46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ciclamato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ciclamato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ciclamato de sódio	12256803	20917	40	1401418
Caelo	Ciclamato de sódio	12105622	21380	40	20120423
Caelo	Ciclamato de sódio	182167	24379	40	20181023*
Caelo	Ciclamato de sódio	20004287009	26234	40	20201216
Caelo	Ciclamato de sódio	20004287009	26234SI	20	20201216
Caelo	Ciclamato de sódio	24002330	27429	40	20241028*
Gatt-Koller	Ciclamato de sódio	23J00242	26702	40	20230308
Gatt-Koller	Ciclamato de sódio	23J00242	26702SI	20	20230308

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 8 reference samples from the substance/substance group *Ciclamato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Ciclamato de sódio*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclamato de sódio	16119302	23259	40
Caelo	Ciclamato de sódio	170411	23853	40
Caelo	Ciclamato de sódio	22003585	26716	40
Caelo	Ciclamato de sódio	22003585	26716SI	20

- 201 944 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 223 spectra from 178 *Apo-Ident* customers from 42 batches from the substance/substance group *Ciclamato de sódio*.

- Among them are spectra of independent samples from 40 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ciclamato de sódio	20004287013	1
	Ciclamato de sódio	20004287014	1
	Ciclamato de sódio	20004287017	3
	Ciclamato de sódio	22003585002	3
	Ciclamato de sódio	22003585006	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ciclamato de sódio	10380915	2
Caelo	Ciclamato de sódio	11204205	1
Caelo	Ciclamato de sódio	14149602	1
Caelo	Ciclamato de sódio	15201601	2
Caelo	Ciclamato de sódio	15201606	2
Caelo	Ciclamato de sódio	15201608	4
Caelo	Ciclamato de sódio	15201614	1
Caelo	Ciclamato de sódio	16119302	4
Caelo	Ciclamato de sódio	16119302/2280217	1
Caelo	Ciclamato de sódio	16119308	8
Caelo	Ciclamato de sódio	16119310	1
Caelo	Ciclamato de sódio	17041102	8
Caelo	Ciclamato de sódio	17362202	7
Caelo	Ciclamato de sódio	17362203	1
Caelo	Ciclamato de sódio	17362207	8
Caelo	Ciclamato de sódio	17362208	8
Caelo	Ciclamato de sódio	179617362207	1
Caelo	Ciclamato de sódio	17961821675	1
Caelo	Ciclamato de sódio	18053101	1
Caelo	Ciclamato de sódio	182167002	6
Caelo	Ciclamato de sódio	182167004	6
Caelo	Ciclamato de sódio	182167005	6
Caelo	Ciclamato de sódio	18216702	9
Caelo	Ciclamato de sódio	18216704	7
Caelo	Ciclamato de sódio	18216707	19
Caelo	Ciclamato de sódio	200004287003	1
Caelo	Ciclamato de sódio	20004278013	1
Caelo	Ciclamato de sódio	20004285001	7
Caelo	Ciclamato de sódio	20004287003	3
Caelo	Ciclamato de sódio	20004287005	6
Caelo	Ciclamato de sódio	20004287007	7
Caelo	Ciclamato de sódio	20004287009	8
Caelo	Ciclamato de sódio	20004287011	4
Caelo	Ciclamato de sódio	20004287013	3
Caelo	Ciclamato de sódio	20004287014	4
Caelo	Ciclamato de sódio	200042887005	1
Caelo	Ciclamato de sódio	22003585002	2
Caelo	Ciclamato de sódio	3092002	1
Caeol/ Noweda	Ciclamato de sódio	16119302	1
Caesar & Loretz GmbH...	Ciclamato de sódio	20004287013	1
Caesar & Loretz GmbH...	Ciclamato de sódio	18216704	1
Caesar & Loretz GmbH...	Ciclamato de sódio	182167004	2
Caesar & Loretz GmbH/AHD	Ciclamato de sódio	20004287013	1
Caesar & Loretz GmbH...	Ciclamato de sódio	182167005	1
Caesar & Loretz GmbH/Gehe	Ciclamato de sódio	20004285001	3
Caesar & Loretz GmbH...	Ciclamato de sódio	20004287003	1
Caesar & Loretz GmbH...	Ciclamato de sódio	20004287007	1
Caesar & Loretz GmbH...	Ciclamato de sódio	20004287014	1
Caesar & Loretz GmbH...	Ciclamato de sódio	20004287007	1
Caesar & Loretz GmbH	Ciclamato de sódio	12105622	1
Caesar & Loretz GmbH	Ciclamato de sódio	17362208	3
Caesar & Loretz GmbH	Ciclamato de sódio	182167002	3
Caesar & Loretz GmbH	Ciclamato de sódio	182167004	4
Caesar & Loretz GmbH	Ciclamato de sódio	182167005	4
Caesar & Loretz GmbH	Ciclamato de sódio	18216702	3
Caesar & Loretz GmbH	Ciclamato de sódio	18216707	4
Caesar & Loretz GmbH	Ciclamato de sódio	20004285001	2
Caesar & Loretz GmbH	Ciclamato de sódio	20004287003	3
Caesar & Loretz GmbH	Ciclamato de sódio	20004287013	1
Caesar & Loretz GmbH	Ciclamato de sódio	20004287014	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar&Loretz GmbH/ …	Ciclamato de sódio	16119308	1
Euro OTC	Ciclamato de sódio	16119302	1
Phoenix	Ciclamato de sódio	20004287014	1
Phoenix	Ciclamato de sódio	22003585002	1
Phoenix	Ciclamato de sódio	787/03100611	1
Phönix	Ciclamato de sódio	182167002	1

- 235 844 spectra from 1515 *Apo-Ident* customers from a total of 49 217 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ciclamato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciclamato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	140	0	201 944
Type C	0	222	1	235 844

The substance/substance group *Ciclamato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	99.5516 % (> 98.2063 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20917	20917	0,00	181,62
21380	20917	17,26	179,20
24379	24379	0,00	184,01
26234	24379	11,94	183,27
26702	27429	47,44	180,26
27429	27429	0,00	184,12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ciclopirox olamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20601-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ciclopirox olamina; Ciclopirox olaminum

Special notes

When selecting the *Ciclopirox olamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ciclopirox olamina	11	4	96

Second-stage model

For differentiation of the substance/substance group *Ciclopirox olamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ciclopirox olamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	83,02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ciclopirox olamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ciclopirox olamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ciclopirox olamina	13343209	21298	40	AR-15-FG-016214-01
Caelo	Ciclopirox olamina	14147406	21655	60	AR-15-FG-014857-01
Caelo	Ciclopirox olamina	14147406	21655SI	60	AR-15-FG-014857-01
Caelo	Ciclopirox olamina	14378809	21991	60	20150227
Caelo	Ciclopirox olamina	14378809	21991SI	60	20150227
Caelo	Ciclopirox olamina	15364408	23011	40	20151201
Caelo	Ciclopirox olamina	15364408	23011SI	40	20151201
Caelo	Ciclopirox olamina	22001499003	26233	40	20220627
Caelo	Ciclopirox olamina	22001499003	26233SI	40	20220627
Caelo	Ciclopirox olamina	24000678	27327	40	20240506*
Caelo	Ciclopirox olamina	24000678	27327SI	40	20240506*
Fagron	Ciclopirox olamina	13A16-N04	21218	40	20130117
Fagron	Ciclopirox olamina	14F13-B03-302340	21964	60	1608170
Fagron	Ciclopirox olamina	14F13-B03-302340	21964SI	60	1608170
Fagron	Ciclopirox olamina	16G26-B02-324884	22969	40	20160907
Fagron	Ciclopirox olamina	16G26-B02-324884	23108	40	20160907
Fagron	Ciclopirox olamina	20B24-F02-370988	25481	40	2102412
Fagron	Ciclopirox olamina	20B24-F02-370988	25481SI	40	2102412
Fagron	Ciclopirox olamina	21B03-B08-210563	25839	50	20210331
Fagron	Ciclopirox olamina	21B03-B08-210563	25839SI	70	20210331

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 960 spectra of 20 reference samples from the substance/substance group *Ciclopirox olamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 002 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 9 reference samples from the substance/substance group *Ciclopirox olamina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclopirox olamina	182102	24280	40
Caelo	Ciclopirox olamina	22003201	26507	40
Fagron	Ciclopirox olamina	14E21-M04	21594	60
Fagron	Ciclopirox olamina	22A11-B03-215669	26176	40
Caelo	Ciclopirox olamina	22003201	26507SI	40
Fagron	Ciclopirox olamina	14E21-M04	21594SI	60
Fagron	Ciclopirox olamina	16G26-B02-324884	22969SI†	40
Fagron	Ciclopirox olamina	16G26-B02-324884	23108SI†	40
Fagron	Ciclopirox olamina	22A11-B03-215669	26176SI	40

- 201 684 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 404 spectra from 171 *Apo-Ident* customers from 102 batches from the substance/substance group *Ciclopirox olamina*.
- Among them are spectra of independent samples from 96 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ciclopirox olamina	22001499004	1
	Ciclopirox olamina	22003201002	1
	Ciclopirox olamina	22003201004	5
	Ciclopirox olamina	22003201009	3
	Ciclopirox olamina	23000858003	1
Cael	Ciclopirox olamina	12040911	2
Caelo	Ciclopirox olamina	12040906	1
Caelo	Ciclopirox olamina	12040911	1
Caelo	Ciclopirox olamina	12B22-N03	1
Caelo	Ciclopirox olamina	13343	1
Caelo	Ciclopirox olamina	13343201	1
Caelo	Ciclopirox olamina	13343203	1
Caelo	Ciclopirox olamina	13343208	2
Caelo	Ciclopirox olamina	13343209	3
Caelo	Ciclopirox olamina	14147402	4
Caelo	Ciclopirox olamina	14147405	1
Caelo	Ciclopirox olamina	14275801	2
Caelo	Ciclopirox olamina	14275802	2
Caelo	Ciclopirox olamina	14378801	2
Caelo	Ciclopirox olamina	14378802	1
Caelo	Ciclopirox olamina	14378803	1
Caelo	Ciclopirox olamina	14378804	2
Caelo	Ciclopirox olamina	14378805	4
Caelo	Ciclopirox olamina	14378806	5
Caelo	Ciclopirox olamina	14378809	3
Caelo	Ciclopirox olamina	14378810	9
Caelo	Ciclopirox olamina	15018802	3
Caelo	Ciclopirox olamina	15018803	2
Caelo	Ciclopirox olamina	15304407	1
Caelo	Ciclopirox olamina	15364402	6
Caelo	Ciclopirox olamina	15364404	2
Caelo	Ciclopirox olamina	15364405	5
Caelo	Ciclopirox olamina	15364407	6
Caelo	Ciclopirox olamina	15364408	4
Caelo	Ciclopirox olamina	15364409	2
Caelo	Ciclopirox olamina	15364412	5
Caelo	Ciclopirox olamina	15364414	1
Caelo	Ciclopirox olamina	15364416	2
Caelo	Ciclopirox olamina	16G26-B02-330862	1
Caelo	Ciclopirox olamina	16G26-B02-337355	3
Caelo	Ciclopirox olamina	17118801	5
Caelo	Ciclopirox olamina	17118802	3
Caelo	Ciclopirox olamina	17118806	11
Caelo	Ciclopirox olamina	17118807	4
Caelo	Ciclopirox olamina	17118808	7
Caelo	Ciclopirox olamina	17118811	4
Caelo	Ciclopirox olamina	17307402	10
Caelo	Ciclopirox olamina	17307403	4
Caelo	Ciclopirox olamina	17307405	6
Caelo	Ciclopirox olamina	173074055727	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ciclopirox olamina	17307408	2
Caelo	Ciclopirox olamina	17307410	8
Caelo	Ciclopirox olamina	1810201	1
Caelo	Ciclopirox olamina	182102002	30
Caelo	Ciclopirox olamina	182102003	6
Caelo	Ciclopirox olamina	182102004	3
Caelo	Ciclopirox olamina	182102007	1
Caelo	Ciclopirox olamina	18210201	17
Caelo	Ciclopirox olamina	18210202	4
Caelo	Ciclopirox olamina	18210203	1
Caelo	Ciclopirox olamina	18210204	1
Caelo	Ciclopirox olamina	18210205	2
Caelo	Ciclopirox olamina	18210209	5
Caelo	Ciclopirox olamina	18210210	14
Caelo	Ciclopirox olamina	18212003	1
Caelo	Ciclopirox olamina	1850000758	1
Caelo	Ciclopirox olamina	21000032002	3
Caelo	Ciclopirox olamina	21000032003	3
Caelo	Ciclopirox olamina	21000032007	2
Caelo	Ciclopirox olamina	21000032008	2
Caelo	Ciclopirox olamina	21000032010	5
Caelo	Ciclopirox olamina	21000032012	1
Caelo	Ciclopirox olamina	21000032015	2
Caelo	Ciclopirox olamina	21000032016	1
Caelo	Ciclopirox olamina	2100032010	1
Caelo	Ciclopirox olamina	21B03-B08-210563	1
Caelo	Ciclopirox olamina	22001499003	5
Caelo	Ciclopirox olamina	22001499004	4
Caelo	Ciclopirox olamina	22001499009	2
Caelo	Ciclopirox olamina	22001499011	2
Caelo	Ciclopirox olamina	22003201002	2
Caelo	Ciclopirox olamina	22003201004	2
Caelo	Ciclopirox olamina	3200003	1
Caesar & Lorenz GmbH	Ciclopirox olamina	171188007	1
Caesar & Loretz GmbH...	Ciclopirox olamina	18210205	1
Caesar & Loretz GmbH...	Ciclopirox olamina	21000032007	1
Caesar & Loretz GmbH/GEHE	Ciclopirox olamina	182102002	1
Caesar & Loretz GmbH/GEHE	Ciclopirox olamina	21000032007	4
Caesar & Loretz GmbH/Gehe	Ciclopirox olamina	22001499004	2
Caesar & Loretz GmbH...	Ciclopirox olamina	21000032008	1
Caesar & Loretz GmbH	Ciclopirox olamina	17307405	1
Caesar & Loretz GmbH	Ciclopirox olamina	17307407	1
Caesar & Loretz GmbH	Ciclopirox olamina	17307410	1
Caesar & Loretz GmbH	Ciclopirox olamina	182102002	6
Caesar & Loretz GmbH	Ciclopirox olamina	182102003	4
Caesar & Loretz GmbH	Ciclopirox olamina	18210201	4
Caesar & Loretz GmbH	Ciclopirox olamina	18210205	1
Caesar & Loretz GmbH	Ciclopirox olamina	18210210	5
Caesar & Loretz GmbH	Ciclopirox olamina	21000032002	4
Caesar & Loretz GmbH	Ciclopirox olamina	21000032003	2
Caesar & Loretz GmbH	Ciclopirox olamina	21000032007	1
Caesar & Loretz GmbH	Ciclopirox olamina	21000032008	2
Caesar & Loretz GmbH	Ciclopirox olamina	21000032010	7
Caesar & Loretz GmbH	Ciclopirox olamina	21000032012	1
Caesar & Loretz GmbH	Ciclopirox olamina	21000032016	2
Caesar & Loretz GmbH	Ciclopirox olamina	22001499004	1
Caesar & Loretz GmbH	Ciclopirox olamina	22001499011	1
Caesar & Loretz GmbH	Ciclopirox olamina	22003201002	1
Caesar & Loretz GmbH	Ciclopirox olamina	22003201004	1
Caesar & Loretz Hild...	Ciclopirox olamina	18210205	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz Hilden	Ciclopirox olamina	17307408	1
Caesar & Loretz Hilden	Ciclopirox olamina	182102002	1
Caesar & Loretz Hilden	Ciclopirox olamina	182102003	1
Cealo	Ciclopirox olamina	14147403	2
Euro OTC	Ciclopirox olamina	14378811	2
Euro OTC	Ciclopirox olamina	17118806	1
Euro OTC	Ciclopirox olamina	1718806	1
Fagron	Ciclopirox olamina	10L09-N03	1
Fagron	Ciclopirox olamina	11h03-n02	1
Fagron	Ciclopirox olamina	12G12-N09	2
Fagron	Ciclopirox olamina	13A16-N04	1
Fagron	Ciclopirox olamina	14378806	1
Fagron	Ciclopirox olamina	14E21-M05	1
Fagron	Ciclopirox olamina	14F13-B03	1
Fagron	Ciclopirox olamina	14F13-B03-302339	1
Fagron	Ciclopirox olamina	16G26-B02	1
Fagron	Ciclopirox olamina	16G26-B02-335198	1
Fagron	Ciclopirox olamina	16G26-B02-348603	1
Fagron	Ciclopirox olamina	19A21-B02-362290	2
Fagron	Ciclopirox olamina	20B24_F02_368880	1
Fagron	Ciclopirox olamina	20B24-F02-372655	1
Fagron	Ciclopirox olamina	21B03B08210563	1
Fagron	Ciclopirox olamina	A160013	1
Fargon/Phönix	Ciclopirox olamina	21B03B08210563	1
Gehe	Ciclopirox olamina	14E21-M04	1
Gehe	Ciclopirox olamina	14F13-B03-302339	1
GEHE	Ciclopirox olamina	15364405	1
Gehe	Ciclopirox olamina	17118808	1
Noweda	Ciclopirox olamina	12040911	1
Noweda	Ciclopirox olamina	12B22-N03	1
Noweda	Ciclopirox olamina	17307404	1
Noweda	Ciclopirox olamina	182102003	1
Noweda	Ciclopirox olamina	18210204	1
Noweda	Ciclopirox olamina	22001499011	1
Pharmachem	Ciclopirox olamina	17118808	1
Phoenix	Ciclopirox olamina	15364412	1
Phönix	Ciclopirox olamina	13A16-N04	1
Phönix	Ciclopirox olamina	17307410	1
Phönix	Ciclopirox olamina	18210209	1
Phönix	Ciclopirox olamina	18210210	2
phönix	Ciclopirox olamina	21000032016	1
Phönix	Ciclopirox olamina	22003201004	1
phönix	Ciclopirox olamina	22003201009	1
Phönix	Ciclopirox olamina	23000858003	2
Sanacorp	Ciclopirox olamina	17118806	1
Sanacorp	Ciclopirox olamina	19A21-B02-362290	1

- 235 663 spectra from 1515 *Apo-Ident* customers from a total of 49 156 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ciclopirox olamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciclopirox olamina* and it was

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	960	0	152 002
Type B	0	400	0	201 684
Type C	0	399	5	235 663

The substance/substance group *Ciclopirox olamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3750 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.7624 % (> 98.0198 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21218	21964	6,87	186,17
21298	21298	0,00	162,72
21655	21655	0,00	170,54
21964	21964	0,00	189,38
21991	21298	7,93	163,37
22969	21964	7,53	183,95
23011	21298	6,81	155,87
23108	21964	6,72	185,22
25481	25481	0,00	145,01
25839	27327	44,69	166,42
26233	21964	23,31	180,47
27327	27327	0,00	165,11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ciclosporina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20941-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ciclosporina; Ciclosporinum

Special notes

When selecting the *Ciclosporina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ciclosporina	7	8	123

Second-stage model

For differentiation of the substance/substance group *Ciclosporina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ciclosporina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	98,78	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ciclosporina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ciclosporina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ciclosporina	13148604	21474	60	1412541
Caelo	Ciclosporina	13148604	21475	60	20130613
Caelo	Ciclosporina	173327	24401	35	20180111*
Caelo	Ciclosporina	192538	25200	40	20191107*
Euro OTC	Ciclosporina	2002031	25356	40	20200825*
Fagron	Ciclosporina	13D26-N07	20941	40	1402057
Fagron	Ciclosporina	13D26-N07	21671	42	1508429
Fagron	Ciclosporina	18G30_B04-354759	24441	40	20181115
Fagron	Ciclosporina	20B13-F03-368652	25182	40	20200313

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 397 spectra of 9 reference samples from the substance/substance group *Ciclosporina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 565 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 383 spectra of 13 reference samples from the substance/substance group *Ciclosporina*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclosporina	12317707	21082	30
Caelo	Ciclosporina	15278907	22966	40
Caelo	Ciclosporina	171583	23669	40
Euro OTC	Ciclosporina	2209015	26342	40
Euro OTC	Ciclosporina	2304018	26772	40
Euro OTC	Ciclosporina	2405004	27363	40
Fagron	Ciclosporina	16C09-B02-325955	23521	30
Fagron	Ciclosporina	23C01-B04-228703	26667	40
Caelo	Ciclosporina	173327	24401†	5
Euro OTC	Ciclosporina	2209015	26342SI	20
Euro OTC	Ciclosporina	2304018	26772SI	20
Fagron	Ciclosporina	13D26-N07	21671†	18
Fagron	Ciclosporina	23C01-B04-228703	26667SI	20

- 201 701 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 440 spectra from 168 *Apo-Ident* customers from 130 batches from the substance/substance group *Ciclosporina*.

- Among them are spectra of independent samples from 123 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ciclosporina	22003878002	14
	Ciclosporina	2203878002	1
	Ciclosporina	23001155005	1
	Ciclosporina	23C01-B04-226120	1
	Ciclosporina	23C01-B04-228702	1
	Ciclosporina	23c01-b04-228703	1
Audor Pharma	Ciclosporina	AP170802HBC	2
Caelo	Ciclosporina	1(192538002)	1
Caelo	Ciclosporina	12165602	3
Caelo	Ciclosporina	12165603	2
Caelo	Ciclosporina	12317702	2
Caelo	Ciclosporina	12317703	1
Caelo	Ciclosporina	12317707	4
Caelo	Ciclosporina	13031303	1
Caelo	Ciclosporina	13031801	1
Caelo	Ciclosporina	13148604	2
Caelo	Ciclosporina	13148606	6
Caelo	Ciclosporina	13346803	3
Caelo	Ciclosporina	13346808	1
Caelo	Ciclosporina	13A28-N04	4
Caelo	Ciclosporina	13D26-N07	4
Caelo	Ciclosporina	14199104	3
Caelo	Ciclosporina	14A15-No1	1
Caelo	Ciclosporina	15049703	4
Caelo	Ciclosporina	15278901	4
Caelo	Ciclosporina	15278902	2
Caelo	Ciclosporina	15278903	3
Caelo	Ciclosporina	15278904	7
Caelo	Ciclosporina	15278910	1
Caelo	Ciclosporina	15278913	1
Caelo	Ciclosporina	15278916	1
Caelo	Ciclosporina	15D23-B05-308853	1
Caelo	Ciclosporina	17158303	7
Caelo	Ciclosporina	17158306	4
Caelo	Ciclosporina	17158309	5
Caelo	Ciclosporina	17332702	6
Caelo	Ciclosporina	17332703	3
Caelo	Ciclosporina	1733702	1
Caelo	Ciclosporina	18041817	1
Caelo	Ciclosporina	18136101	8
Caelo	Ciclosporina	18136104	14
Caelo	Ciclosporina	18136108	5
Caelo	Ciclosporina	19011301	1
Caelo	Ciclosporina	19055803	1
Caelo	Ciclosporina	19055804	18
Caelo	Ciclosporina	19055805	14
Caelo	Ciclosporina	19055807	1
Caelo	Ciclosporina	19055808	2
Caelo	Ciclosporina	19055809	1
Caelo	Ciclosporina	19055810	1
Caelo	Ciclosporina	192538002	9
Caelo	Ciclosporina	192538004	1
Caelo	Ciclosporina	192538005	4
Caelo	Ciclosporina	192538007	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ciclosporina	20E08-F06-371274	1
Caelo	Ciclosporina	21000144001	1
Caelo	Ciclosporina	21000144002	12
Caelo	Ciclosporina	21000144010	8
Caelo	Ciclosporina	21000144012	4
Caelo	Ciclosporina	21000144013	1
Caelo	Ciclosporina	2100144012	1
Caelo	Ciclosporina	21A25-F02-376839	1
Caelo	Ciclosporina	29689114C22B02	1
Caesar & Loretz GmbH...	Ciclosporina	19055805	1
Caesar & Loretz GmbH...	Ciclosporina	21000144010	2
Caesar & Loretz GmbH...	Ciclosporina	192538002	1
Caesar & Loretz GmbH...	Ciclosporina	192538002	1
Caesar & Loretz GmbH...	Ciclosporina	21000144002	1
Caesar & Loretz GmbH	Ciclosporina	17332702	1
Caesar & Loretz GmbH	Ciclosporina	18136104	6
Caesar & Loretz GmbH	Ciclosporina	19055804	1
Caesar & Loretz GmbH	Ciclosporina	19055805	8
Caesar & Loretz GmbH	Ciclosporina	192538002	10
Caesar & Loretz GmbH	Ciclosporina	192538007	6
Caesar & Loretz GmbH	Ciclosporina	21000144002	5
Caesar & Loretz GmbH	Ciclosporina	21000144004	1
Caesar & Loretz GmbH	Ciclosporina	21000144010	5
Caesar & Loretz GmbH	Ciclosporina	21000144011	1
Caesar & Loretz GmbH	Ciclosporina	21000144012	4
Caesar & Loretz GmbH	Ciclosporina	21000941001	1
Caesar & Loretz GmbH	Ciclosporina	F06-3712702	1
Caesar & Loretz	Ciclosporina	17158306	1
Concord Biotech Ltd....	Ciclosporina	14G22-B02-296891	1
Euro OTC	Ciclosporina	256866	1
Fagron	Ciclosporina	10J18-N06	1
Fagron	Ciclosporina	1103531	1
Fagron	Ciclosporina	11K17-N13	1
Fagron	Ciclosporina	12E31-N02	7
Fagron	Ciclosporina	13414038	1
Fagron	Ciclosporina	13417083	2
Fagron	Ciclosporina	13420003	1
Fagron	Ciclosporina	13420023	4
Fagron	Ciclosporina	13420107	1
Fagron	Ciclosporina	13421135	1
Fagron	Ciclosporina	13A28-n04	1
Fagron	Ciclosporina	13A28-N04	4
Fagron	Ciclosporina	13B19N02	2
Fagron	Ciclosporina	13B19-N02	4
Fagron	Ciclosporina	13d026N07	1
Fagron	Ciclosporina	13D26-N07	10
Fagron	Ciclosporina	13H19_N09	1
Fagron	Ciclosporina	13H19-N09	4
Fagron	Ciclosporina	14/18-B02-300180	1
Fagron	Ciclosporina	14718-b02-300180	1
Fagron	Ciclosporina	14a15-n01	1
Fagron	Ciclosporina	14A15-N01	3
Fagron	Ciclosporina	14g22-b02-296891	1
Fagron	Ciclosporina	14G22-B02-296891	5
Fagron	Ciclosporina	15D23-B05	2
Fagron	Ciclosporina	15D23-B05-307217	1
Fagron	Ciclosporina	15D23-B05-308853	7
Fagron	Ciclosporina	15F29-B14	1
Fagron	Ciclosporina	15f29-b14-316270	2
Fagron	Ciclosporina	15F29B14316270	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ciclosporina	15F29-B14-316270	1
Fagron	Ciclosporina	15F29-B14-321791	1
Fagron	Ciclosporina	15f29-b14-325654	1
Fagron	Ciclosporina	16121401	1
Fagron	Ciclosporina	18136104	1
Fagron	Ciclosporina	18A18-B07-344620	3
Fagron	Ciclosporina	18A18-B07-344621	1
Fagron	Ciclosporina	18A18-B07-344622	1
Fagron	Ciclosporina	18A18-B07-349163	2
Fagron	Ciclosporina	18G30-B04	3
Fagron	Ciclosporina	18G30-B04-0001	1
Fagron	Ciclosporina	18G30-B04-354758	1
Fagron	Ciclosporina	18G30-B04-354759	4
Fagron	Ciclosporina	18G30-B04-3568304	1
Fagron	Ciclosporina	18G30-B04-358809	3
Fagron	Ciclosporina	20B13-F03	2
Fagron	Ciclosporina	20B13-F03-368653	1
Fagron	Ciclosporina	20E08-F06-3124	1
Fagron	Ciclosporina	20E08-F06-371272	2
Fagron	Ciclosporina	20E08-F06-371273	7
Fagron	Ciclosporina	20E08-F06-371275	2
Fagron	Ciclosporina	21A25-F02-376839	2
Fagron	Ciclosporina	21J12-B19-216847	1
Fagron	Ciclosporina	21J12-B19-217253	2
Fagron	Ciclosporina	21K15-B05-215789	3
Fagron	Ciclosporina	21K15-B05-216970	2
Fagron	Ciclosporina	21K15-B05-217761	1
Fagron	Ciclosporina	21L14-B02-219484	2
Fagron	Ciclosporina	21L14-B02-221862	2
Fagron	Ciclosporina	23C01-B04-223807	1
Fagron	Ciclosporina	23C01-B04-226120	2
Fagron	Ciclosporina	25051302	1
Fagron	Ciclosporina	59865-13-3	1
Fargon/Gehe	Ciclosporina	18A18-B07-344620	1
Fargon	Ciclosporina	13D26-No7	1
Gehe	Ciclosporina	17158303	1
Gehe	Ciclosporina	17158306	1
Gehe	Ciclosporina	17332702	1
Gehe	Ciclosporina	17332703	1
Gehe	Ciclosporina	18136101	1
Gehe	Ciclosporina	18136104	1
Gehe	Ciclosporina	22003878002	2
Gehe	Ciclosporina	23001155005	1
Medisca/Ortscheidt	Ciclosporina		1
Noweda	Ciclosporina	23C01-B04-231019	1
Ortscheid 21.10.2021	Ciclosporina		1
Phoenix	Ciclosporina	17158303	1
Phoenix	Ciclosporina	20B13-F03-368653	1
Phönix	Ciclosporina	13D26-N07	1
Sanacorp	Ciclosporina	21000144002	2
Sanacorp	Ciclosporina	23C01-B04-226120	1
VDL	Ciclosporina	13D26-N07	1

- 235 627 spectra from 1515 *Apo-Ident* customers from a total of 49 131 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ciclosporina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciclosporina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	397	0	152 565
Type B	0	383	0	201 701
Type C	0	438	2	235 627

The substance/substance group *Ciclosporina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4887 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4334 %)
Type C	100.0000 % (> 99.9007 %)	99.5455 % (> 98.8636 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20941	20941	0,00	119,69
21474	21474	0,00	129,12
21475	21474	2,89	129,00
21671	21671	0,00	121,50
24401	24401	0,00	128,60
24441	21474	16,07	127,95
25182	20941	13,17	122,19
25200	25200	0,00	127,35
25356	25356	0,00	114,42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cistina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20515-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cistina

Special notes

When selecting the *Cistina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cistina	8	5	15

Second-stage model

For differentiation of the substance/substance group *Cistina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cistina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de lisina	83,37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cistina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cistina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cistina	1307052-01	21328	40	20130918
Euro OTC	Cistina	1408016-01	21715	60	20140911
Euro OTC	Cistina	1603010	22523	40	20160406*
Euro OTC	Cistina	1610013	22863	40	20161110*
Euro OTC	Cistina	1801016	23879	40	20180126*
Euro OTC	Cistina	2009038	25411	40	20201020*
Euro OTC	Cistina	2305001	26876	40	20230802*
Fagron	Cistina	15F08-B05-310685	23767	40	20150616

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 340 spectra of 8 reference samples from the substance/substance group *Cistina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 622 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 230 spectra of 7 reference samples from the substance/substance group *Cistina*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cistina	1811005	24332	40
Euro OTC	Cistina	1904022	24617	40
Euro OTC	Cistina	1910028	24933	40
Euro OTC	Cistina	2202004	26036	40
Euro OTC	Cistina	2207020	26435	40
Euro OTC	Cistina	2202004	26036SI	10
Euro OTC	Cistina	2305001	26876SI†	20

- 201 854 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 9 *Apo-Ident* customers from 16 batches from the substance/substance group *Cistina*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cistina	190402201	1
Euro OTC	Cistina	1204090	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cistina	1207013-01	2
Euro OTC	Cistina	1801016-01	3
Euro OTC	Cistina	1811005-01	2
Euro OTC	Cistina	1904022-01	1
Euro OTC	Cistina	1910028-01	1
Euro OTC	Cistina	2009038-01	4
Euro OTC	Cistina	2009038-02	3
Euro OTC	Cistina	2081301	1
Euro OTC	Cistina	2202004-01	3
Euro OTC	Cistina	26081408	1
Euro OTC	Cistina	30041809	1
Euro OTC	Cistina	3021502	1
Fagron	Cistina	12D26-B04-285823	2
Fagron	Cistina	15F08-B05-310685	1
Fagron	Cistina	1904022-01	1
Fagron	Cistina	1910028-01	3

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cistina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cistina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	230	0	201 854
Type C	0	32	0	236 035

The substance/substance group *Cistina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.3913 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.2500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21328	23879	5,84	137,53
21715	22523	5,26	136,70
22523	22523	0,00	138,53
22863	22863	0,00	141,69
23767	23879	12,20	141,71
23879	23879	0,00	140,07
25411	25411	0,00	136,69
26876	26876	0,00	152,48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de cafeína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20701-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de cafeína; Coffeini citras

Special notes

When selecting the *Citrato de cafeína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de cafeína	5	2	30

Second-stage model

For differentiation of the substance/substance group *Citrato de cafeína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de cafeína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	111,91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de cafeína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de cafeína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Citrato de cafeína	12C16-N03	20701	40	1403477
Fagron	Citrato de cafeína	15A05-B03-318006	22530	40	20150115
Fagron	Citrato de cafeína	15A05-B03-318006	22531	40	20150115
Gatt-Koller	Citrato de cafeína	1783/05140715	21844	60	AR-15-FG-014994-01
Gatt-Koller	Citrato de cafeína	22J00881	26626	40	20220718
Gatt-Koller	Citrato de cafeína	23J02625	27092	40	20240130
Gatt-Koller	Citrato de cafeína	23J02625	27092SI	20	20240130

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Citrato de cafeína*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 682 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Citrato de cafeína*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Citrato de cafeína	15A05-B03-302746	21734	60
Gatt-Koller	Citrato de cafeína	4065/11164916	23112	40
Fagron	Citrato de cafeína	15A05-B03-302746	22729	40
Gatt-Koller	Citrato de cafeína	22J00881	26626SI†	20

- 201 924 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 82 spectra from 55 *Apo-Ident* customers from 34 batches from the substance/substance group *Citrato de cafeína*.
- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD	Citrato de cafeína	13B08-N02	1
Caelo	Citrato de cafeína	11F21-N05	1
Caelo	Citrato de cafeína	13D30-N02	1
Caelo	Citrato de cafeína	15A05-B03-302746	1
Caelo	Citrato de cafeína	15A05-B03-307309	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de cafeína	15A05-B03-318006	2
Fagron	Citrato de cafeína	10c23-n02	1
Fagron	Citrato de cafeína	10H02-N02	2
Fagron	Citrato de cafeína	11082015A	1
Fagron	Citrato de cafeína	11C29-N04	2
Fagron	Citrato de cafeína	12C16-N03	1
Fagron	Citrato de cafeína	12J05-N06	3
Fagron	Citrato de cafeína	12J05-N06	1
Fagron	Citrato de cafeína	13B08N02	1
Fagron	Citrato de cafeína	13B08-N02	1
Fagron	Citrato de cafeína	13D30-N02	9
Fagron	Citrato de cafeína	13D30-No2	1
Fagron	Citrato de cafeína	15A05B03	1
Fagron	Citrato de cafeína	15A05-B03	3
Fagron	Citrato de cafeína	15a05-b03-302746	1
Fagron	Citrato de cafeína	15A05-B03-302746	11
Fagron	Citrato de cafeína	15A05-B03-307135	3
Fagron	Citrato de cafeína	15a05-b03-318006	1
Fagron	Citrato de cafeína	15A05-B03-318006	11
Fagron	Citrato de cafeína	2002311282	1
Fagron	Citrato de cafeína	204311282	1
Fagron	Citrato de cafeína	26021401	1
Fagron	Citrato de cafeína	2714E-01282	1
Fagron	Citrato de cafeína	2813E1282	1
Fagron	Citrato de cafeína	3314E-01282	1
Fagron	Citrato de cafeína	3513I-01282	1
Fagron	Citrato de cafeína	3914U-01282	1
Fagron	Citrato de cafeína	4213U01282	1
Fagron	Citrato de cafeína	5013U01282	1
Fagron	Citrato de cafeína	CCC1205	1
Fagron	Citrato de cafeína	CCD-1401	3
Fargon/Phoenix	Citrato de cafeína	15A05-B03-302746	1
Fargon	Citrato de cafeína	12J05-N06	1
Fgron	Citrato de cafeína	2013Q-01282	1
Gehe	Citrato de cafeína	13B08-N02	1
Noweda	Citrato de cafeína	CCC-1101	1
Phoenix	Citrato de cafeína	15A05-B03	1
Rondell Apotheke	Citrato de cafeína	15A05-B03-307309	1

- 235 985 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de cafeína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato de cafeína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	160	0	201 924
Type C	0	72	10	235 985

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Citrato de cafeína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	87.8049 % (> 84.1463 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20701	20701	0,00	342,93
21844	21844	0,00	279,24
22530	20701	24,26	343,26
22531	20701	29,21	343,94
26626	21844	102,51	262,52
27092	21844	100,50	292,99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de cálcio tetra-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20013-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de cálcio tetra-hidratado

Special notes

When selecting the *Citrato de cálcio tetra-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de cálcio tetra-hidratado	8	10	129

Second-stage model

For differentiation of the substance/substance group *Citrato de cálcio tetra-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de cálcio tetra-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	73,70	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de cálcio tetra-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de cálcio tetra-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citrato de cálcio tetra-h…	13391203	21320	40	20131205
Caelo	Citrato de cálcio tetra-h…	13391203	21486	40	20131205
Caelo	Citrato de cálcio tetra-h…	171768	23651	40	20170713*
Euro OTC	Citrato de cálcio tetra-h…	1305018-01	21249	40	20130528
Euro OTC	Citrato de cálcio tetra-h…	1509039	21931	60	20151013*
Euro OTC	Citrato de cálcio tetra-h…	1509039-01	22255	60	20151013
Euro OTC	Citrato de cálcio tetra-h…	1701001	22995	40	20170124*
Euro OTC	Citrato de cálcio tetra-h…	2206009	26184	40	20220624*
Euro OTC	Citrato de cálcio tetra-h…	2206009	26184SI	20	20220624*
Euro OTC	Citrato de cálcio tetra-h…	2305020	26748	40	20230607*
Euro OTC	Citrato de cálcio tetra-h…	2305020	26748SI	20	20230607*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Citrato de cálcio tetra-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 522 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 11 reference samples from the substance/substance group *Citrato de cálcio tetra-hidratado*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citrato de cálcio tetra-h…	181608	24230	40
Caelo	Citrato de cálcio tetra-h…	20002273	25287	40
Caelo	Citrato de cálcio tetra-h…	21004151	26124	40
Caelo	Citrato de cálcio tetra-h…	24001206	27230	40
Euro OTC	Citrato de cálcio tetra-h…	1606001	22681	40
Euro OTC	Citrato de cálcio tetra-h…	1707025	23606	40
Euro OTC	Citrato de cálcio tetra-h…	1803031	24077	40
Euro OTC	Citrato de cálcio tetra-h…	1901002	24514	40
Euro OTC	Citrato de cálcio tetra-h…	1912013	25075	40
Euro OTC	Citrato de cálcio tetra-h…	2105004	25769	50
Caelo	Citrato de cálcio tetra-h…	21004151	26124SI	20

- 201 654 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 330 spectra from 146 *Apo-Ident* customers from 135 batches from the substance/substance group *Citrato de cálcio tetra-hidratado*.

- Among them are spectra of independent samples from 129 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citrato de cálcio tetra-h…	21004151003	2
	Citrato de cálcio tetra-h…	21004151004	1
	Citrato de cálcio tetra-h…	21004151009	1
8,35Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	20002273013	1
ACM	Citrato de cálcio tetra-h…	KNC0740J15	1
Alliance Health 23.1…	Citrato de cálcio tetra-h…	1402003-01	1
Alliance Healthcare	Citrato de cálcio tetra-h…	20002273006	2
Caelo	Citrato de cálcio tetra-h…		2
Caelo	Citrato de cálcio tetra-h…	11061402	1
Caelo	Citrato de cálcio tetra-h…	11168803	1
Caelo	Citrato de cálcio tetra-h…	11168806	3
Caelo	Citrato de cálcio tetra-h…	11168813	1
Caelo	Citrato de cálcio tetra-h…	1119E-01209	1
Caelo	Citrato de cálcio tetra-h…	11349301	1
Caelo	Citrato de cálcio tetra-h…	11349304	2
Caelo	Citrato de cálcio tetra-h…	11349309	2
Caelo	Citrato de cálcio tetra-h…	11349313	2
Caelo	Citrato de cálcio tetra-h…	11349318	3
Caelo	Citrato de cálcio tetra-h…	11349320	1
Caelo	Citrato de cálcio tetra-h…	11349325	2
Caelo	Citrato de cálcio tetra-h…	1168806	1
Caelo	Citrato de cálcio tetra-h…	1168813	1
Caelo	Citrato de cálcio tetra-h…	12310401	1
Caelo	Citrato de cálcio tetra-h…	12310402	2
Caelo	Citrato de cálcio tetra-h…	12310403	3
Caelo	Citrato de cálcio tetra-h…	12310406	5
Caelo	Citrato de cálcio tetra-h…	12310407	2
Caelo	Citrato de cálcio tetra-h…	12310411	2
Caelo	Citrato de cálcio tetra-h…	12310413	4
Caelo	Citrato de cálcio tetra-h…	12310417	3
Caelo	Citrato de cálcio tetra-h…	12310418	2
Caelo	Citrato de cálcio tetra-h…	13391203	4
Caelo	Citrato de cálcio tetra-h…	133912042x	1
Caelo	Citrato de cálcio tetra-h…	13391205	5
Caelo	Citrato de cálcio tetra-h…	1408017-01	1
Caelo	Citrato de cálcio tetra-h…	14133303	1
Caelo	Citrato de cálcio tetra-h…	14133307	1
Caelo	Citrato de cálcio tetra-h…	14133310	1
Caelo	Citrato de cálcio tetra-h…	1509039-01	1
Caelo	Citrato de cálcio tetra-h…	1509039-02	1
Caelo	Citrato de cálcio tetra-h…	15177701	1
Caelo	Citrato de cálcio tetra-h…	15177702	2
Caelo	Citrato de cálcio tetra-h…	15177703	7
Caelo	Citrato de cálcio tetra-h…	15375702	6
Caelo	Citrato de cálcio tetra-h…	15375703	1
Caelo	Citrato de cálcio tetra-h…	15375707	1
Caelo	Citrato de cálcio tetra-h…	15375712	2
Caelo	Citrato de cálcio tetra-h…	15375713	6
Caelo	Citrato de cálcio tetra-h…	1600565	1
Caelo	Citrato de cálcio tetra-h…	16021502	1
Caelo	Citrato de cálcio tetra-h…	16056501	1
Caelo	Citrato de cálcio tetra-h…	16056504	4
Caelo	Citrato de cálcio tetra-h…	16056505	3
Caelo	Citrato de cálcio tetra-h…	16056510	2
Caelo	Citrato de cálcio tetra-h…	1606001-02	1
Caelo	Citrato de cálcio tetra-h…	1705038-01	1
Caelo	Citrato de cálcio tetra-h…	1707025-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de cálcio tetra-h…	1716803	1
Caelo	Citrato de cálcio tetra-h…	1716808	1
Caelo	Citrato de cálcio tetra-h…	17176803	6
Caelo	Citrato de cálcio tetra-h…	17176805	1
Caelo	Citrato de cálcio tetra-h…	17176806	6
Caelo	Citrato de cálcio tetra-h…	17176808	7
Caelo	Citrato de cálcio tetra-h…	17176812	3
Caelo	Citrato de cálcio tetra-h…	17176816	1
Caelo	Citrato de cálcio tetra-h…	17176818	1
Caelo	Citrato de cálcio tetra-h…	18160802	3
Caelo	Citrato de cálcio tetra-h…	18160803	1
Caelo	Citrato de cálcio tetra-h…	18160805	1
Caelo	Citrato de cálcio tetra-h…	18160811	1
Caelo	Citrato de cálcio tetra-h…	18160813	2
Caelo	Citrato de cálcio tetra-h…	19010002-01	1
Caelo	Citrato de cálcio tetra-h…	19061315	1
Caelo	Citrato de cálcio tetra-h…	20002273004	2
Caelo	Citrato de cálcio tetra-h…	20002273009	2
Caelo	Citrato de cálcio tetra-h…	20002273010	1
Caelo	Citrato de cálcio tetra-h…	20002273013	2
Caelo	Citrato de cálcio tetra-h…	2000227306	1
Caelo	Citrato de cálcio tetra-h…	2001377004	1
Caelo	Citrato de cálcio tetra-h…	2016Q-01209	1
Caelo	Citrato de cálcio tetra-h…	21001377004	1
Caelo	Citrato de cálcio tetra-h…	21004151002	1
Caelo	Citrato de cálcio tetra-h…	2114M1209	1
Caelo	Citrato de cálcio tetra-h…	3512U-01209	1
Caelo	Citrato de cálcio tetra-h…	71356168	1
Caelo	Citrato de cálcio tetra-h…	92192429	1
Caelo	Citrato de cálcio tetra-h…	92457399	1
Caesar & Loretz GmbH…	Citrato de cálcio tetra-h…	20002273013	1
Caesar & Loretz GmbH…	Citrato de cálcio tetra-h…	18160811	1
Caesar & Loretz GmbH…	Citrato de cálcio tetra-h…	181608002	3
Caesar & Loretz GmbH…	Citrato de cálcio tetra-h…	21001377004	1
Caesar & Loretz GmbH…	Citrato de cálcio tetra-h…	21004151002	2
Caesar & Loretz GmbH/OG	Citrato de cálcio tetra-h…	20002273002	1
Caesar & Loretz GmbH…	Citrato de cálcio tetra-h…	20002273010	1
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	17176814	1
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	181608002	3
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	18160802	3
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	18160804	3
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	18160811	1
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	18160812	3
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	18160813	1
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	20002273002	2
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	20002273004	3
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	20002273009	3
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	20002273013	1
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	21001377004	1
Caesar & Loretz GmbH	Citrato de cálcio tetra-h…	21001377009	1
Caesar & Loretz	Citrato de cálcio tetra-h…	16056509	1
Cealo	Citrato de cálcio tetra-h…	12310401	1
Dr.Lohmann	Citrato de cálcio tetra-h…	3042527	1
EuRho/Jenne	Citrato de cálcio tetra-h…	1211007-01	1
EuRho	Citrato de cálcio tetra-h…	1502012-02	1
euro ct	Citrato de cálcio tetra-h…	1912013-01	5
Euro OTC	Citrato de cálcio tetra-h…	1009030-01	1
Euro OTC	Citrato de cálcio tetra-h…	1058904	1
Euro OTC	Citrato de cálcio tetra-h…	1207006-01	2
Euro OTC	Citrato de cálcio tetra-h…	1211007-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Citrato de cálcio tetra-h…	13031204	1
Euro OTC	Citrato de cálcio tetra-h…	1305018-01	3
Euro OTC	Citrato de cálcio tetra-h…	1305018-02	1
Euro OTC	Citrato de cálcio tetra-h…	1402003-01	2
Euro OTC	Citrato de cálcio tetra-h…	140801701	1
Euro OTC	Citrato de cálcio tetra-h…	1408017-01	4
Euro OTC	Citrato de cálcio tetra-h…	1502012-01	1
Euro OTC	Citrato de cálcio tetra-h…	1502021-02	1
Euro OTC	Citrato de cálcio tetra-h…	1509039-01	4
Euro OTC	Citrato de cálcio tetra-h…	1509039-02	6
Euro OTC	Citrato de cálcio tetra-h…	15177704	1
Euro OTC	Citrato de cálcio tetra-h…	1606001-01	1
Euro OTC	Citrato de cálcio tetra-h…	1606001-02	2
Euro OTC	Citrato de cálcio tetra-h…	1701001-01	2
Euro OTC	Citrato de cálcio tetra-h…	1701001-02	1
Euro OTC	Citrato de cálcio tetra-h…	1707025-01	3
Euro OTC	Citrato de cálcio tetra-h…	1707025-02	2
Euro OTC	Citrato de cálcio tetra-h…	1707025-41	1
Euro OTC	Citrato de cálcio tetra-h…	1710007-01	1
Euro OTC	Citrato de cálcio tetra-h…	1803031-01	3
Euro OTC	Citrato de cálcio tetra-h…	1803031-02	7
Euro OTC	Citrato de cálcio tetra-h…	190100201	1
Euro OTC	Citrato de cálcio tetra-h…	1901002-01	6
Euro OTC	Citrato de cálcio tetra-h…	1901002-02	4
Euro OTC	Citrato de cálcio tetra-h…	191201301	1
Euro OTC	Citrato de cálcio tetra-h…	1912013-01	12
Euro OTC	Citrato de cálcio tetra-h…	1912013-02	6
Euro OTC	Citrato de cálcio tetra-h…	1912013-13	1
Euro OTC	Citrato de cálcio tetra-h…	2105004-01	3
Euro OTC	Citrato de cálcio tetra-h…	2817U-01209	1
Euro OTC	Citrato de cálcio tetra-h…	3006222	1
Euro OTC	Citrato de cálcio tetra-h…	3037086	1
Euro OTC	Citrato de cálcio tetra-h…	3842527	1
Fagron	Citrato de cálcio tetra-h…	13d16-n06	1
Fagron	Citrato de cálcio tetra-h…	13D16-N06	1
Fagron	Citrato de cálcio tetra-h…	150903901	1
Gatt-Koller	Citrato de cálcio tetra-h…	1802139	3
Gehe Kassel	Citrato de cálcio tetra-h…	14133307	1
Gehe	Citrato de cálcio tetra-h…	18160806	1
Gehe	Citrato de cálcio tetra-h…	21001377009	1
Krieger	Citrato de cálcio tetra-h…	17176808	1
L12	Citrato de cálcio tetra-h…	1606001-03	1
lohmann	Citrato de cálcio tetra-h…	3045397	1
Noweda	Citrato de cálcio tetra-h…	1509039-01	1
Noweda	Citrato de cálcio tetra-h…	17176803	1
Noweda	Citrato de cálcio tetra-h…	17176808	1
Noweda	Citrato de cálcio tetra-h…	18160804	1
Noweda	Citrato de cálcio tetra-h…	18160813	1
Noweda	Citrato de cálcio tetra-h…	20002273004	1
Phönix	Citrato de cálcio tetra-h…	1305018-01	1
Sanacorp WE: 12.08.1…	Citrato de cálcio tetra-h…	711105	1
Sanacorp	Citrato de cálcio tetra-h…	1211007-01	1
Sanacorp	Citrato de cálcio tetra-h…	14133310	1
Sanacorp	Citrato de cálcio tetra-h…	20002273002	1

- 235 737 spectra from 1515 *Apo-Ident* customers from a total of 49 126 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de cálcio tetra-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato de cálcio tetra-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	430	0	201 654
Type C	0	330	0	235 737

The substance/substance group *Citrato de cálcio tetra-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.1818 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21249	22995	6,17	101,73
21320	22995	7,49	105,13
21486	22995	7,26	105,83
21931	21931	0,00	96,86
22255	21931	4,74	97,82
22995	22995	0,00	101,06
23651	23651	0,00	101,68
26184	26184	0,00	101,99
26748	26748	0,00	101,93

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de fentanila**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21164-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de fentanila; Fentanila, citrato; Fentanyli citras

Special notes

When selecting the *Citrato de fentanila* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de fentanila	3	1	21

Second-stage model

For differentiation of the substance/substance group *Citrato de fentanila* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de fentanila* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	114,76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de fentanila* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de fentanila*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Citrato de fentanila	13G30-N06	21164	40	0814M-07678
Fagron	Citrato de fentanila	13G30-N06	21164SI	60	0814M-07678
Fagron	Citrato de fentanila	15F18-B01-525098	22431	60	1316R-03686
Fagron	Citrato de fentanila	15F18-B01-525098	22431SI	60	1316R-03686
Fagron	Citrato de fentanila	15F18-B01-525166	22432	60	1316Q-03686
Fagron	Citrato de fentanila	15F18-B01-525166	22432SI	60	1316Q-03686

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 340 spectra of 6 reference samples from the substance/substance group *Citrato de fentanila*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 622 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Citrato de fentanila*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Citrato de fentanila	16E26-B01-525360	23480	40
Fagron	Citrato de fentanila	16E26-B01-525360	23480SI	40

- 202 004 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 23 spectra from 13 *Apo-Ident* customers from 21 batches from the substance/substance group *Citrato de fentanila*.
- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Citrato de fentanila	10H20-N02	1
Fagron	Citrato de fentanila	14J03-B06-525002	1
Fagron	Citrato de fentanila	14Jo3-B06-525002	1
Fagron	Citrato de fentanila	16E26-B01-525231	1
Fagron	Citrato de fentanila	16E26-B01-525232	1
Fagron	Citrato de fentanila	16J06-B03-525432	1
Fagron	Citrato de fentanila	17L14-B04-525639	1
Fagron	Citrato de fentanila	17L14-B04-525660	1
Fagron	Citrato de fentanila	18B12-B06	1
Fagron	Citrato de fentanila	18L27-B03-525913	1
Fagron	Citrato de fentanila	18L27-B03-525914	2
Fagron	Citrato de fentanila	19-00252	1
Fagron	Citrato de fentanila	19D09-B04-525979	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Citrato de fentanila	19E27-K04	1
Fagron	Citrato de fentanila	19K21-F025	1
Fagron	Citrato de fentanila	19K21-F02-526085	2
Fagron	Citrato de fentanila	20100911-1	1
Fagron	Citrato de fentanila	20E20-F12	1
Fagron	Citrato de fentanila	20E20-F12-526324	1
Fagron	Citrato de fentanila	20E28-K01	1
Fargon/Gehe	Citrato de fentanila	21A19-K01	1

- 236 044 spectra from 1515 *Apo-Ident* customers from a total of 49 237 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de fentanila* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato de fentanila* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	80	0	202 004
Type C	0	20	3	236 044

The substance/substance group *Citrato de fentanila* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	86.9565 % (> 73.9130 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21164	21164	0,00	159,21
22431	22431	0,00	155,31
22432	22432	0,00	153,76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de magnésio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20616-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de magnésio; Magnesii citras

Special notes

When selecting the *Citrato de magnésio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de magnésio	13	6	18

Second-stage model

For differentiation of the substance/substance group *Citrato de magnésio* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de magnésio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	39,04	39,20
Sulfato de polimixina B	40,69	–
Cromoglicato de sódio	63,43	–
⋮	⋮	⋮
Carbômero	66,36	63,43
Sulfato de gentamicina	>50	103,36
Gluconato de zinco	>50	147,96
Tetraborato de sódio	>50	156,36
Fosfato de Mg-Ca-K-colamina	>50	170,28
Sulfato de tobramicina	>50	202,41
Sulfato de neomicina	>50	215,38
Finasterida	>50	940,06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de magnésio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de magnésio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Citrato de magnésio	1501031	21794	60	AR-15-FG-007845-01
Euro OTC	Citrato de magnésio	1506020	21829	60	20150623*
Euro OTC	Citrato de magnésio	1507019	21860	60	20150722*
Euro OTC	Citrato de magnésio	1511018	22225	60	20151130*
Euro OTC	Citrato de magnésio	1602028	22505	40	20160314*
Euro OTC	Citrato de magnésio	1706007	23549	40	20170720*
Euro OTC	Citrato de magnésio	1711018	23895	40	20171129*
Euro OTC	Citrato de magnésio	1803033	24088	40	20180403*
Euro OTC	Citrato de magnésio	1808020	24202	40	20180827*
Euro OTC	Citrato de magnésio	1902006	24480	40	20190226*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Citrato de magnésio	2003051	25170	40	20200428*
Euro OTC	Citrato de magnésio	2012001	25465	40	20201216*
Euro OTC	Citrato de magnésio	2105003	25708	50	20210701*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 610 spectra of 13 reference samples from the substance/substance group *Citrato de magnésio*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 352 spectra from a total of 2829 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 8 reference samples from the substance/substance group *Citrato de magnésio*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Citrato de magnésio	1607006	22673	40
Euro OTC	Citrato de magnésio	1701018	22998	40
Euro OTC	Citrato de magnésio	1810026	24308	40
Euro OTC	Citrato de magnésio	1907040	24778	40
Euro OTC	Citrato de magnésio	2212004	26530	40
Euro OTC	Citrato de magnésio	2404010	27210	40
Euro OTC	Citrato de magnésio	2212004	26530SI	20
Euro OTC	Citrato de magnésio	2404010	27210SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 804 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 25 *Apo-Ident* customers from 18 batches from the substance/substance group *Citrato de magnésio*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citrato de magnésio	2105003-01	1
	Citrato de magnésio	2401010-01	1
AHD	Citrato de magnésio	2212004-01	1
APOrtha Deutschland GmbH	Citrato de magnésio	17000809/0	1
Arktis	Citrato de magnésio	894P/2418	1
Caelo	Citrato de magnésio	1701018-01	1
Euro OTC	Citrato de magnésio	1602028-01	1
Euro OTC	Citrato de magnésio	1706007-01	3
Euro OTC	Citrato de magnésio	1711018-01	2
Euro OTC	Citrato de magnésio	1808020-01	2
Euro OTC	Citrato de magnésio	180820-01	1
Euro OTC	Citrato de magnésio	1810026-01	2
Euro OTC	Citrato de magnésio	1902006-01	3
Euro OTC	Citrato de magnésio	1907040-01	4
Euro OTC	Citrato de magnésio	2003051-01	3
Euro OTC	Citrato de magnésio	2012001-01	1
Euro OTC	Citrato de magnésio	2105003-01	1
Euro OTC	Citrato de magnésio	3060884	2
Euro OTC	Citrato de magnésio	3086441	1

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de magnésio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato de magnésio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	610	0	152 352
Type B	0	280	0	201 804
Type C	0	32	0	236 035

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Citrato de magnésio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0164 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.2500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21794	21794	0,00	60,63
21829	21829	0,00	99,18
21860	21860	0,00	88,96
22225	22225	0,00	77,32
22505	22505	0,00	83,94
23549	23549	0,00	46,66
23895	23895	0,00	86,90
24088	24088	0,00	98,75
24202	24202	0,00	111,16
24480	24480	0,00	59,03
25170	25170	0,00	60,95
25465	25465	0,00	55,37
25708	25708	0,00	48,63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20021-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de potássio; Citrato de potássio monoidratado

Special notes

When selecting the *Citrato de potássio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de potássio	11	14	171

Second-stage model

For differentiation of the substance/substance group *Citrato de potássio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	86,37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citrato de potássio	11320212	20655	40	20111201
Caelo	Citrato de potássio	13317618	21452	60	20130926
Caelo	Citrato de potássio	15123103	21775	60	20150414
Caelo	Citrato de potássio	161130	22476	60	20160602*
Caelo	Citrato de potássio	21000107	25558	40	20210113*
Caelo	Citrato de potássio	22002808	26481	40	20221104*
Caelo	Citrato de potássio	22002808	26481SI	20	20221104*
Euro OTC	Citrato de potássio	1509044	21936	60	20151013*
Euro OTC	Citrato de potássio	1611017	22921	40	20161207*
Euro OTC	Citrato de potássio	1912008	25090	40	20200115*
Euro OTC	Citrato de potássio	2101026	25607	40	20210126*
Euro OTC	Citrato de potássio	2105012	25703	50	20210630*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 12 reference samples from the substance/substance group *Citrato de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 412 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 600 spectra of 16 reference samples from the substance/substance group *Citrato de potássio*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citrato de potássio	170929	23290	40
Caelo	Citrato de potássio	180385	24046	40
Caelo	Citrato de potássio	191804	24736	40
Euro OTC	Citrato de potássio	1603040	22521	40
Euro OTC	Citrato de potássio	1606041	22676	40
Euro OTC	Citrato de potássio	1705024	23428	40
Euro OTC	Citrato de potássio	1803003	24084	40
Euro OTC	Citrato de potássio	1807034	24160	40
Euro OTC	Citrato de potássio	1902027	24485	40
Euro OTC	Citrato de potássio	1907016	24785	40
Euro OTC	Citrato de potássio	2008015	25346	40
Euro OTC	Citrato de potássio	2109025	25881	50
Euro OTC	Citrato de potássio	2212005	26535	40
Euro OTC	Citrato de potássio	2311001	27006	40
Euro OTC	Citrato de potássio	2109025	25881SI	10
Euro OTC	Citrato de potássio	2212005	26535SI	20

- 201 484 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 522 spectra from 232 *Apo-Ident* customers from 177 batches from the substance/substance group *Citrato de potássio*.
- Among them are spectra of independent samples from 171 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citrato de potássio		1
	Citrato de potássio	123345	1
	Citrato de potássio	12345	1
	Citrato de potássio	22002808006	1
	Citrato de potássio	2212005-01	5
	Citrato de potássio	24000093002	1
	Citrato de potássio	24000093005	1
	Citrato de potássio	hfdf5545	1
ACM	Citrato de potássio	KNC0196J15	4
Alliance/EurRho	Citrato de potássio	3055187	1
Alliance	Citrato de potássio	1611017-01	1
Caelo	Citrato de potássio		9
Caelo	Citrato de potássio	11102201	1
Caelo	Citrato de potássio	1112008-01	1
Caelo	Citrato de potássio	11320201	1
Caelo	Citrato de potássio	11320212	3
Caelo	Citrato de potássio	116I-01737	1
Caelo	Citrato de potássio	1204016-01	1
Caelo	Citrato de potássio	12135302	6
Caelo	Citrato de potássio	12135303	2
Caelo	Citrato de potássio	12135309	2
Caelo	Citrato de potássio	12135311	1
Caelo	Citrato de potássio	1215309	1
Caelo	Citrato de potássio	12299201	5
Caelo	Citrato de potássio	12299202	1
Caelo	Citrato de potássio	12299203	4
Caelo	Citrato de potássio	12334	1
Caelo	Citrato de potássio	1234	4
Caelo	Citrato de potássio	12345	3
Caelo	Citrato de potássio	12345678	1
Caelo	Citrato de potássio	123654879	1
Caelo	Citrato de potássio	123test	2
Caelo	Citrato de potássio	123Test	4
Caelo	Citrato de potássio	123Testmessung	1
Caelo	Citrato de potássio	12456	1
Caelo	Citrato de potássio	1256369	1
Caelo	Citrato de potássio	12648	1
Caelo	Citrato de potássio	13080602	8
Caelo	Citrato de potássio	13080603	1
Caelo	Citrato de potássio	13135902	1
Caelo	Citrato de potássio	13135904	1
Caelo	Citrato de potássio	13135907	5
Caelo	Citrato de potássio	13135908	1
Caelo	Citrato de potássio	1314M-01737	1
Caelo	Citrato de potássio	13317602	2
Caelo	Citrato de potássio	13317603	2
Caelo	Citrato de potássio	13317604	2
Caelo	Citrato de potássio	13317613	3
Caelo	Citrato de potássio	13317618	2
Caelo	Citrato de potássio	14138105	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de potássio	14138107	1
Caelo	Citrato de potássio	14138112	1
Caelo	Citrato de potássio	14138118	3
Caelo	Citrato de potássio	14138119	1
Caelo	Citrato de potássio	151231	1
Caelo	Citrato de potássio	15123102	2
Caelo	Citrato de potássio	15123103	4
Caelo	Citrato de potássio	15148701	7
Caelo	Citrato de potássio	15148702	1
Caelo	Citrato de potássio	15148706	11
Caelo	Citrato de potássio	15148707	4
Caelo	Citrato de potássio	15148708	2
Caelo	Citrato de potássio	15158706	1
Caelo	Citrato de potássio	15434709	1
Caelo	Citrato de potássio	154357	3
Caelo	Citrato de potássio	15435701	7
Caelo	Citrato de potássio	15435702	1
Caelo	Citrato de potássio	154357025	1
Caelo	Citrato de potássio	15435703	5
Caelo	Citrato de potássio	15435709	3
Caelo	Citrato de potássio	15435710	5
Caelo	Citrato de potássio	15435711	1
Caelo	Citrato de potássio	1543702	1
Caelo	Citrato de potássio	15896	1
Caelo	Citrato de potássio	16113002	3
Caelo	Citrato de potássio	16113003	2
Caelo	Citrato de potássio	16113006	6
Caelo	Citrato de potássio	16113007	3
Caelo	Citrato de potássio	16113008	2
Caelo	Citrato de potássio	16113012	10
Caelo	Citrato de potássio	17061402	1
Caelo	Citrato de potássio	170922904	1
Caelo	Citrato de potássio	17092903	8
Caelo	Citrato de potássio	17092904	5
Caelo	Citrato de potássio	18007603	3
Caelo	Citrato de potássio	18007604	2
Caelo	Citrato de potássio	18007607	2
Caelo	Citrato de potássio	18038502	3
Caelo	Citrato de potássio	18038506	11
Caelo	Citrato de potássio	18038507	2
Caelo	Citrato de potássio	18038509	1
Caelo	Citrato de potássio	18038512	2
Caelo	Citrato de potássio	18038514	5
Caelo	Citrato de potássio	18038517	3
Caelo	Citrato de potássio	18038519	4
Caelo	Citrato de potássio	18038523	1
Caelo	Citrato de potássio	1807034-01	1
Caelo	Citrato de potássio	189645	1
Caelo	Citrato de potássio	191804001	5
Caelo	Citrato de potássio	191804006	6
Caelo	Citrato de potássio	191804008	1
Caelo	Citrato de potássio	191804009	2
Caelo	Citrato de potássio	191804011	1
Caelo	Citrato de potássio	19180402	2
Caelo	Citrato de potássio	20004139002	2
Caelo	Citrato de potássio	20004139003	4
Caelo	Citrato de potássio	21000107002	2
Caelo	Citrato de potássio	21000107005	1
Caelo	Citrato de potássio	21000107010	4
Caelo	Citrato de potássio	21000107015	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de potássio	2114M1737	1
Caelo	Citrato de potássio	232262310107	1
Caelo	Citrato de potássio	26113006	1
Caelo	Citrato de potássio	28021402	1
Caelo	Citrato de potássio	3012Q-01737	1
Caelo	Citrato de potássio	3094247	1
Caelo	Citrato de potássio	3112M01737	1
Caelo	Citrato de potássio	3456	1
Caelo	Citrato de potássio	3618E-01737	1
Caelo	Citrato de potássio	411025-1-P	1
Caelo	Citrato de potássio	5021509	1
Caelo	Citrato de potássio	5555	1
Caelo	Citrato de potássio	71730128	2
Caelo	Citrato de potássio	71730367	1
Caelo	Citrato de potássio	9259107	1
Caelo	Citrato de potássio	9259120	1
Caelo	Citrato de potássio	Caelo	1
Caelo	Citrato de potássio	gfte	1
Caelo	Citrato de potássio	RT115113	1
Caesar & Loretz GmbH...	Citrato de potássio	19180402	1
Caesar & Loretz GmbH...	Citrato de potássio	18038519	1
Caesar & Loretz GmbH...	Citrato de potássio	19180402	1
Caesar & Loretz GmbH...	Citrato de potássio	191804006	1
Caesar & Loretz GmbH/Gehe	Citrato de potássio	191804011	1
Caesar & Loretz GmbH...	Citrato de potássio	191804009	1
Caesar & Loretz GmbH...	Citrato de potássio	21000107001	1
Caesar & Loretz GmbH...	Citrato de potássio	21000107003	1
Caesar & Loretz GmbH/Ph	Citrato de potássio	191804006	1
Caesar & Loretz GmbH	Citrato de potássio	18007607	1
Caesar & Loretz GmbH	Citrato de potássio	18038509	1
Caesar & Loretz GmbH	Citrato de potássio	18038514	1
Caesar & Loretz GmbH	Citrato de potássio	191804006	1
Caesar & Loretz GmbH	Citrato de potássio	191804008	1
Caesar & Loretz GmbH	Citrato de potássio	19180401	1
Caesar & Loretz GmbH	Citrato de potássio	191804011	1
Caesar & Loretz GmbH	Citrato de potássio	19180402	7
Caesar & Loretz GmbH	Citrato de potássio	20004139002	1
Caesar & Loretz GmbH	Citrato de potássio	20004139003	1
Caesar & Loretz GmbH	Citrato de potássio	21000107024	1
EuRho/Phoenix	Citrato de potássio	2105012-01	1
EuRho/Phönix	Citrato de potássio	1311036-01	1
EuRho	Citrato de potássio	1603040-01	1
Eurho	Citrato de potássio	2101026-01	1
Euro OT/Phönix	Citrato de potássio	3036325	1
Euro OTC	Citrato de potássio	123456	6
Euro OTC	Citrato de potássio	1306032-01	1
Euro OTC	Citrato de potássio	1311036-01	9
Euro OTC	Citrato de potássio	1406025-01	1
Euro OTC	Citrato de potássio	1410014-01	2
Euro OTC	Citrato de potássio	1504024-01	2
Euro OTC	Citrato de potássio	1509044-01	6
Euro OTC	Citrato de potássio	1603040-01	12
Euro OTC	Citrato de potássio	160601-01	1
Euro OTC	Citrato de potássio	160604-01	1
Euro OTC	Citrato de potássio	160604101	1
Euro OTC	Citrato de potássio	1606041-01	4
Euro OTC	Citrato de potássio	1611017	1
Euro OTC	Citrato de potássio	1611017-01	8
Euro OTC	Citrato de potássio	16113012	1
Euro OTC	Citrato de potássio	1705024-01	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Citrato de potássio	1803003-01	2
Euro OTC	Citrato de potássio	180703401	1
Euro OTC	Citrato de potássio	1807034-01	8
Euro OTC	Citrato de potássio	1902027	1
Euro OTC	Citrato de potássio	1902027-01	7
Euro OTC	Citrato de potássio	190227-01	1
Euro OTC	Citrato de potássio	190701601	2
Euro OTC	Citrato de potássio	1907016-01	2
Euro OTC	Citrato de potássio	191200-01	1
Euro OTC	Citrato de potássio	1912008-01	9
Euro OTC	Citrato de potássio	1912008-02	4
Euro OTC	Citrato de potássio	1915A-01737	1
Euro OTC	Citrato de potássio	192027-01	1
Euro OTC	Citrato de potássio	20004139003	1
Euro OTC	Citrato de potássio	2008015-01	7
Euro OTC	Citrato de potássio	2008015-02	4
Euro OTC	Citrato de potássio	2008015-15	1
Euro OTC	Citrato de potássio	2101026-01	6
Euro OTC	Citrato de potássio	2105012-01	6
Euro OTC	Citrato de potássio	2109025-01	8
Euro OTC	Citrato de potássio	2109025-02	2
Euro OTC	Citrato de potássio	22101303	1
Euro OTC	Citrato de potássio	3126221	1
EuRoh/Noweda	Citrato de potássio	1807034-01	1
Fagron	Citrato de potássio		1
Fagron	Citrato de potássio	1234567	1
Fragon/ Gehe	Citrato de potássio	3055187	1
Gatt-Koller	Citrato de potássio	1800758	1
Gehe	Citrato de potássio	19180402	1
ghfgh	Citrato de potássio	3654645	1
Gutenberg-Apotheke	Citrato de potássio	13135907	1
Hiperscan	Citrato de potássio		1
HiperScan	Citrato de potássio		1
L12	Citrato de potássio	15435709	1
Labor	Citrato de potássio	1234	2
lohmann	Citrato de potássio	1051470	1
Nachprüfung	Citrato de potássio	111112	1
Nachprüfung	Citrato de potássio	123456	1
Noweda 10.12.2019	Citrato de potássio	18007607	1
Noweda	Citrato de potássio	18038506	1
Noweda	Citrato de potássio	21000107014	1
Phoenix 08.07.2014	Citrato de potássio	13317624	1
Phoenix Goettin	Citrato de potássio	13317613	1
Phoenix	Citrato de potássio	1326PLV-1739	1
Phoenix	Citrato de potássio	15148708	1
Phönix	Citrato de potássio	1211006-01	2
Phönix	Citrato de potássio	15123103	1
Sanacorb	Citrato de potássio	12135311	2
Sanacorp/ euRho	Citrato de potássio	1204016-01	1
Sanacorp	Citrato de potássio	14138105	1
Sanacorp	Citrato de potássio	160604101	1
Sanacorp	Citrato de potássio	191804006	1
Test	Citrato de potássio	12345	1
Testsubstanz	Citrato de potássio		1

- 235 545 spectra from 1515 *Apo-Ident* customers from a total of 49 094 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	550	0	152 412
Type B	0	600	0	201 484
Type C	0	515	7	235 545

The substance/substance group *Citrato de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9091 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.6590 % (> 98.0843 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20655	21936	5,41	263,28
21452	22476	8,45	261,47
21775	21936	5,44	263,63
21936	21936	0,00	259,90
22476	22476	0,00	262,76
22921	22921	0,00	258,38
25090	25090	0,00	263,09
25558	25558	0,00	266,30
25607	25607	0,00	257,96
25703	25703	0,00	257,83
26481	26481	0,00	267,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de sildenafila**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20852-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de sildenafila; Sildenafila, citrato; Sildenafili citras

Special notes

When selecting the *Citrato de sildenafila* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de sildenafila	7	10	197

Second-stage model

For differentiation of the substance/substance group *Citrato de sildenafila* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de sildenafila* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	101,23	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de sildenafila* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de sildenafila*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citrato de sildenafila	160498	22446	60	20160307*
Caelo	Citrato de sildenafila	170715	23336	40	20170529*
Caelo	Citrato de sildenafila	170715	23345	40	20170529*
Euro OTC	Citrato de sildenafila	1311010-01	21621	60	20131209
Euro OTC	Citrato de sildenafila	1311010-04	23178	40	20150309
Euro OTC	Citrato de sildenafila	1908006	24843	40	20190906*
Fagron	Citrato de sildenafila	13F24-N03	20852	40	1402052
Fagron	Citrato de sildenafila	13J15-N01	20927	80	20131030

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 400 spectra of 8 reference samples from the substance/substance group *Citrato de sildenafila*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 562 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 14 reference samples from the substance/substance group *Citrato de sildenafila*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citrato de sildenafila	190866	24545	40
Caelo	Citrato de sildenafila	22000907	26248	40
Caelo	Citrato de sildenafila	23003271	27247	40
Euro OTC	Citrato de sildenafila	1807037	24192	40
Euro OTC	Citrato de sildenafila	1902031	24469	40
Euro OTC	Citrato de sildenafila	2003003	25380	40
Euro OTC	Citrato de sildenafila	2111002	25896	50
Euro OTC	Citrato de sildenafila	2301014	26580	40
Euro OTC	Citrato de sildenafila	2403010	27287	40
Fagron	Citrato de sildenafila	21G10-B25-219206	26072	40
Caelo	Citrato de sildenafila	22000907	26248SI	20
Euro OTC	Citrato de sildenafila	2111002	25896SI	50
Euro OTC	Citrato de sildenafila	2301014	26580SI	20
Fagron	Citrato de sildenafila	21G10-B25-219206	26072SI	40

- 201 544 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 743 spectra from 178 *Apo-Ident* customers from 206 batches from the substance/substance group *Citrato de sildenafila*.

- Among them are spectra of independent samples from 196 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citrato de sildenafila	1311010-04	2
	Citrato de sildenafila	2111002-01	1
	Citrato de sildenafila	22000907002	2
	Citrato de sildenafila	22000907012	2
	Citrato de sildenafila	22000907015	5
	Citrato de sildenafila	22000907016	3
	Citrato de sildenafila	22000907018	3
	Citrato de sildenafila	23000811001	5
	Citrato de sildenafila	23000811003	2
	Citrato de sildenafila	23003271003	2
	Citrato de sildenafila	2301014-01	5
	Citrato de sildenafila	23L11-B05-236845	1
	Citrato de sildenafila	7-22792004	1
	Citrato de sildenafila	B07-2279203	1
	Citrato de sildenafila	SLC/0221061	1
	Citrato de sildenafila	SLC/1123066	1
AHC	Citrato de sildenafila	21B17-B09-203496	2
AHC	Citrato de sildenafila	23003271003	1
AHC	Citrato de sildenafila	2301014-01	1
Alliance	Citrato de sildenafila		1
Alliance	Citrato de sildenafila	1311010-03	1
Caelo	Citrato de sildenafila		1
Caelo	Citrato de sildenafila	101051528	1
Caelo	Citrato de sildenafila	1311010-06	1
Caelo	Citrato de sildenafila	14074703	2
Caelo	Citrato de sildenafila	14074707	2
Caelo	Citrato de sildenafila	14074709	1
Caelo	Citrato de sildenafila	14074714	5
Caelo	Citrato de sildenafila	14074715	5
Caelo	Citrato de sildenafila	14074716	1
Caelo	Citrato de sildenafila	1407474	1
Caelo	Citrato de sildenafila	15097301	1
Caelo	Citrato de sildenafila	15097302	1
Caelo	Citrato de sildenafila	15097303	1
Caelo	Citrato de sildenafila	15097306	1
Caelo	Citrato de sildenafila	15097307	2
Caelo	Citrato de sildenafila	15097308	1
Caelo	Citrato de sildenafila	15097310	3
Caelo	Citrato de sildenafila	15097311	1
Caelo	Citrato de sildenafila	15097312	2
Caelo	Citrato de sildenafila	15097315	1
Caelo	Citrato de sildenafila	15097317	2
Caelo	Citrato de sildenafila	15F11-B02-309081	1
Caelo	Citrato de sildenafila	15F11-B02-314725	1
Caelo	Citrato de sildenafila	16049801	1
Caelo	Citrato de sildenafila	16049802	10
Caelo	Citrato de sildenafila	16049805	1
Caelo	Citrato de sildenafila	16049808	4
Caelo	Citrato de sildenafila	16049810	2
Caelo	Citrato de sildenafila	16049811	1
Caelo	Citrato de sildenafila	16049812	1
Caelo	Citrato de sildenafila	16049814	9
Caelo	Citrato de sildenafila	16049819	1
Caelo	Citrato de sildenafila	16049820	5
Caelo	Citrato de sildenafila	16049821	13
Caelo	Citrato de sildenafila	16049823	2
Caelo	Citrato de sildenafila	16049824	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de sildenafila	16049826	1
Caelo	Citrato de sildenafila	16F30-B02-3241715	1
Caelo	Citrato de sildenafila	17071502	2
Caelo	Citrato de sildenafila	17071503	7
Caelo	Citrato de sildenafila	17071504	21
Caelo	Citrato de sildenafila	17344001	2
Caelo	Citrato de sildenafila	17344003	11
Caelo	Citrato de sildenafila	17344004	2
Caelo	Citrato de sildenafila	17344005	9
Caelo	Citrato de sildenafila	17344006	2
Caelo	Citrato de sildenafila	17344008	4
Caelo	Citrato de sildenafila	17344009	3
Caelo	Citrato de sildenafila	1734401	1
Caelo	Citrato de sildenafila	17344010	2
Caelo	Citrato de sildenafila	17344014	3
Caelo	Citrato de sildenafila	17344015	1
Caelo	Citrato de sildenafila	18B13-B06-349160	2
Caelo	Citrato de sildenafila	18B13-B06-351981	1
Caelo	Citrato de sildenafila	1908006-01	2
Caelo	Citrato de sildenafila	1908006-02	1
Caelo	Citrato de sildenafila	190866001	2
Caelo	Citrato de sildenafila	190866005	2
Caelo	Citrato de sildenafila	19086603	3
Caelo	Citrato de sildenafila	19086604	8
Caelo	Citrato de sildenafila	19086605	12
Caelo	Citrato de sildenafila	19086605P-191112-1	1
Caelo	Citrato de sildenafila	19086605P-191212-1	1
Caelo	Citrato de sildenafila	19086605P-200107-1	1
Caelo	Citrato de sildenafila	19086605P-200206-2	1
Caelo	Citrato de sildenafila	19086606	10
Caelo	Citrato de sildenafila	19086606P-200319-5	1
Caelo	Citrato de sildenafila	19086607	2
Caelo	Citrato de sildenafila	190866606	1
Caelo	Citrato de sildenafila	2000016003	1
Caelo	Citrato de sildenafila	20000163002	9
Caelo	Citrato de sildenafila	20000163002/01	1
Caelo	Citrato de sildenafila	20000163003	5
Caelo	Citrato de sildenafila	20000163005	1
Caelo	Citrato de sildenafila	20000163006	3
Caelo	Citrato de sildenafila	2000163003	2
Caelo	Citrato de sildenafila	20004485002	2
Caelo	Citrato de sildenafila	20004485003	7
Caelo	Citrato de sildenafila	21000810001	6
Caelo	Citrato de sildenafila	21000810002	2
Caelo	Citrato de sildenafila	21000810003	6
Caelo	Citrato de sildenafila	21000810004	3
Caelo	Citrato de sildenafila	21000810006	2
Caelo	Citrato de sildenafila	21000810008	3
Caelo	Citrato de sildenafila	21000810010	4
Caelo	Citrato de sildenafila	21000810011	2
Caelo	Citrato de sildenafila	21000810012	1
Caelo	Citrato de sildenafila	2100081008	1
Caelo	Citrato de sildenafila	2100810006	1
Caelo	Citrato de sildenafila	2101403	1
Caelo	Citrato de sildenafila	22000907001	3
Caelo	Citrato de sildenafila	22000907002	6
Caelo	Citrato de sildenafila	22000907008	1
Caelo	Citrato de sildenafila	22000907012	1
Caelo	Citrato de sildenafila	2200090907015	1
Caelo	Citrato de sildenafila	2200907002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de sildenafila	46049826	1
Caelo	Citrato de sildenafila	SLC/0420004	1
Caesar & Loretz GmbH...	Citrato de sildenafila	21000810008	1
Caesar & Loretz GmbH...	Citrato de sildenafila	22000907002	2
Caesar & Loretz GmbH...	Citrato de sildenafila	20004485003	1
Caesar & Loretz GmbH/Gehe	Citrato de sildenafila	19086607	3
Caesar & Loretz GmbH...	Citrato de sildenafila	190866001	2
Caesar & Loretz GmbH...	Citrato de sildenafila	20000163003	2
Caesar & Loretz GmbH...	Citrato de sildenafila	21000810008	1
Caesar & Loretz GmbH...	Citrato de sildenafila	21000810013	1
Caesar & Loretz GmbH...	Citrato de sildenafila	21000810003	1
Caesar & Loretz GmbH...	Citrato de sildenafila	190866003	1
Caesar & Loretz GmbH...	Citrato de sildenafila	20000163004	6
Caesar & Loretz GmbH/Sana	Citrato de sildenafila	19086604	1
Caesar & Loretz GmbH...	Citrato de sildenafila	21000810006	1
Caesar & Loretz GmbH...	Citrato de sildenafila	21000810011	1
Caesar & Loretz GmbH...	Citrato de sildenafila	22000907002	1
Caesar & Loretz GmbH	Citrato de sildenafila	17344013	1
Caesar & Loretz GmbH	Citrato de sildenafila	17344014	1
Caesar & Loretz GmbH	Citrato de sildenafila	180737-01	1
Caesar & Loretz GmbH	Citrato de sildenafila	190866005	1
Caesar & Loretz GmbH	Citrato de sildenafila	19086601	1
Caesar & Loretz GmbH	Citrato de sildenafila	19086603	1
Caesar & Loretz GmbH	Citrato de sildenafila	19086605	1
Caesar & Loretz GmbH	Citrato de sildenafila	19086606	10
Caesar & Loretz GmbH	Citrato de sildenafila	19086607	2
Caesar & Loretz GmbH	Citrato de sildenafila	20000163002	3
Caesar & Loretz GmbH	Citrato de sildenafila	20004485003	3
Caesar & Loretz GmbH	Citrato de sildenafila	21000810003	7
Caesar & Loretz GmbH	Citrato de sildenafila	21000810004	1
Caesar & Loretz GmbH	Citrato de sildenafila	21000810006	5
Caesar & Loretz GmbH	Citrato de sildenafila	21000810007	1
Caesar & Loretz GmbH	Citrato de sildenafila	21000810008	1
Caesar & Loretz GmbH	Citrato de sildenafila	21000810011	1
Caesar & Loretz GmbH	Citrato de sildenafila	21000810012	4
Caesar & Loretz GmbH	Citrato de sildenafila	21000810013	2
Caesar & Loretz GmbH	Citrato de sildenafila	21000810014	2
Caesar & Loretz GmbH	Citrato de sildenafila	2100081003	1
Caesar & Loretz GmbH	Citrato de sildenafila	22000907001	6
Caesar & Loretz GmbH	Citrato de sildenafila	22000907002	4
Caesar & Loretz GmbH	Citrato de sildenafila	22000907012	2
Caesar & Loretz GmbH	Citrato de sildenafila	22000907013	2
Caesar & Loretz GmbH	Citrato de sildenafila	22000907018	1
Caesar & Loretz GmbH	Citrato de sildenafila	B01-2018201	1
Cealo	Citrato de sildenafila	16049805	1
Cealo	Citrato de sildenafila	20000163005	1
Eu Rho	Citrato de sildenafila	1902031-01	1
Eu Rho	Citrato de sildenafila	1908006-01	1
EuRho/Noweda	Citrato de sildenafila	1807037-01	3
EuRho	Citrato de sildenafila	2111002-01	2
Euro OTC	Citrato de sildenafila		1
Euro OTC	Citrato de sildenafila	10061706	1
Euro OTC	Citrato de sildenafila	101031827	1
Euro OTC	Citrato de sildenafila	103031328	1
Euro OTC	Citrato de sildenafila	13110-01	1
Euro OTC	Citrato de sildenafila	1311010	1
Euro OTC	Citrato de sildenafila	1311010-01	4
Euro OTC	Citrato de sildenafila	1311010-02	2
Euro OTC	Citrato de sildenafila	131101003	1
Euro OTC	Citrato de sildenafila	1311010-03	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Citrato de sildenafila	131101004	1
Euro OTC	Citrato de sildenafila	1311010-04	3
Euro OTC	Citrato de sildenafila	1311010-05	6
Euro OTC	Citrato de sildenafila	1311010-06	11
Euro OTC	Citrato de sildenafila	1311010-07	1
Euro OTC	Citrato de sildenafila	1311010-6	1
Euro OTC	Citrato de sildenafila	14051402	1
Euro OTC	Citrato de sildenafila	15081830	1
Euro OTC	Citrato de sildenafila	15097301	1
Euro OTC	Citrato de sildenafila	17061405	1
Euro OTC	Citrato de sildenafila	17081504	1
Euro OTC	Citrato de sildenafila	1807037-01	19
Euro OTC	Citrato de sildenafila	1807037-01x2	1
Euro OTC	Citrato de sildenafila	19011907	1
Euro OTC	Citrato de sildenafila	1902031-01	30
Euro OTC	Citrato de sildenafila	19080006-01	1
Euro OTC	Citrato de sildenafila	1908006-01	22
Euro OTC	Citrato de sildenafila	1908006-02	9
Euro OTC	Citrato de sildenafila	19b07-b02-191473	1
Euro OTC	Citrato de sildenafila	2003003-01	17
Euro OTC	Citrato de sildenafila	2003003-02	12
Euro OTC	Citrato de sildenafila	2111002-01	19
Euro OTC	Citrato de sildenafila	2111002-1	1
Euro OTC	Citrato de sildenafila	2301014-01	2
Euro OTC	Citrato de sildenafila	27021802	1
Euro OTC	Citrato de sildenafila	311010-06	1
Euro OTC	Citrato de sildenafila	5117Q-03684	1
Euro	Citrato de sildenafila	1311010-06	1
Euro	Citrato de sildenafila	190020031-01	1
euro	Citrato de sildenafila	1908006-01	2
Fagron	Citrato de sildenafila	13J15-N01	2
Fagron	Citrato de sildenafila	14H11-B01-303183	1
Fagron	Citrato de sildenafila	15F11-B02	2
Fagron	Citrato de sildenafila	15F11-B02-314725	1
Fagron	Citrato de sildenafila	15f11-b02-320186	1
Fagron	Citrato de sildenafila	15F11-B02-320186	1
Fagron	Citrato de sildenafila	15F11-B02-525175	3
Fagron	Citrato de sildenafila	16049812	1
Fagron	Citrato de sildenafila	16049817	1
Fagron	Citrato de sildenafila	16049819	2
Fagron	Citrato de sildenafila	16A18-B08	2
Fagron	Citrato de sildenafila	16F30-B02	1
Fagron	Citrato de sildenafila	16F30-B02-324715	3
Fagron	Citrato de sildenafila	16F30-B02-331449	1
Fagron	Citrato de sildenafila	16F30-B02-331450	4
Fagron	Citrato de sildenafila	16F30-B02-334977	2
Fagron	Citrato de sildenafila	16F30-B02-324715	1
Fagron	Citrato de sildenafila	17071505	1
Fagron	Citrato de sildenafila	17H31-B02-342459	4
Fagron	Citrato de sildenafila	18B13-B06	1
Fagron	Citrato de sildenafila	18B13-B06-347389	2
Fagron	Citrato de sildenafila	18B13-B06-348000	1
Fagron	Citrato de sildenafila	18B13-B06-348001	2
Fagron	Citrato de sildenafila	18B13-B06-349160	2
Fagron	Citrato de sildenafila	18B13-B06-351981	1
Fagron	Citrato de sildenafila	18B13-B06-353827	1
Fagron	Citrato de sildenafila	19807-B02-194729	1
Fagron	Citrato de sildenafila	19807-B02-194730	1
Fagron	Citrato de sildenafila	19B07-802-194730	1
Fagron	Citrato de sildenafila	19B07-B02-191472	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Citrato de sildenafila	19B07-B02-191473	4
Fagron	Citrato de sildenafila	19B07-B02-191474	1
Fagron	Citrato de sildenafila	19B07-B02-194728	2
Fagron	Citrato de sildenafila	19B07-B02-194729	2
Fagron	Citrato de sildenafila	19K12-B01-195593	1
Fagron	Citrato de sildenafila	19K12-B01-195594	6
Fagron	Citrato de sildenafila	19K12-B01-195594	1
Fagron	Citrato de sildenafila	19K12-B01-195595	1
Fagron	Citrato de sildenafila	20J26-B01-201822	7
Fagron	Citrato de sildenafila	20J26-B01-202653	1
Fagron	Citrato de sildenafila	21B17-B09-203496	3
Fagron	Citrato de sildenafila	21G10-B25	1
Fagron	Citrato de sildenafila	21G10-B25-219206	2
Fagron	Citrato de sildenafila	20J26-B01-201823	1
Fagron	Citrato de sildenafila	B01-2018202	2
Fagron	Citrato de sildenafila	B09-2034906	1
Fargon	Citrato de sildenafila	19B07-B02-194727	2
Gehe	Citrato de sildenafila	13F24-N03	1
Gehe	Citrato de sildenafila	16049805	1
GEHE	Citrato de sildenafila	17344003	1
Gehe	Citrato de sildenafila	17344008	1
Gehe	Citrato de sildenafila	19086606	2
Gutenberg-Apotheke	Citrato de sildenafila	1311010-01	1
Jenne	Citrato de sildenafila	22000907015	1
Noweda/ Caesar & Lor…	Citrato de sildenafila	19086607	1
Noweda	Citrato de sildenafila	18B13-B06-347389	1
Noweda	Citrato de sildenafila	18B13-B06-348002	1
Noweda	Citrato de sildenafila	19086603	1
Noweda	Citrato de sildenafila	19086607	1
Noweda	Citrato de sildenafila	19B07-B02-194728	1
Noweda	Citrato de sildenafila	19B07-B02-191473	1
Noweda	Citrato de sildenafila	SLC/0518011	1
ph euro	Citrato de sildenafila	1908006-02	2
Phoenix	Citrato de sildenafila	1311010-04	2
Phoenix	Citrato de sildenafila	22000907015	1
Phönix	Citrato de sildenafila	2003003-01	1
Phönix	Citrato de sildenafila	22000907018	1
Phönix	Citrato de sildenafila	473102016SC	1
Phönx/Polpharma	Citrato de sildenafila	1311010-01	1
Polpharma/Phoenix	Citrato de sildenafila	131101001	1
Sanacorp WE 21.04.17…	Citrato de sildenafila	16049808	1
Sanacorp	Citrato de sildenafila	14H11-B01-297519	2
Sanacorp	Citrato de sildenafila	16049811	2
Sanacorp	Citrato de sildenafila	19B07-b02-191473	1
Sanacorp	Citrato de sildenafila	2003003-02	1
Sanacorp	Citrato de sildenafila	2111002-01	1
Shangei tengben Biot…	Citrato de sildenafila	20200110	1

- 235 324 spectra from 1515 *Apo-Ident* customers from a total of 49 053 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de sildenafila* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

all relevant spectra of the various substances were compared with *Citrato de sildenafila* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	540	0	201 544
Type C	0	742	1	235 324

The substance/substance group *Citrato de sildenafila* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	99.8654 % (> 99.4616 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20852	20852	0,00	189,80
20927	20852	10,71	191,11
21621	24843	13,09	188,90
22446	22446	0,00	192,33
23178	23336	25,92	193,04
23336	23336	0,00	195,54
23345	23345	0,00	192,75
24843	24843	0,00	191,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20662-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato de sódio; Natrii citras

Special notes

When selecting the *Citrato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato de sódio	11	19	411

Second-stage model

For differentiation of the substance/substance group *Citrato de sódio* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	50,17	–
⋮	⋮	⋮
Capsaicina	>50	137,69
Heparina sódica	>50	173,89
Sacarose	>50	221,71
Cloridrato de quinina di-hidratado	>50	256,66
Piridoxal-5-fosfato	>50	304,46
Levocarnitina	>50	333,14
Cloridrato de oxibutinina	>50	348,28
Amifampridina	>50	429,64
Alfaestradiol	>50	435,17
Prednicarbato	>50	504,61
Cloridrato de ciprofloxacina	>50	594,85
Triclosan	>50	613,22
Metoxisaleno	>50	651,06
Tetracaína	>50	773,85
Acetato de ciproterona	>50	1008,42
Acetato de noretisterona	>50	1165,10
Cloridrato de amitriptilina	>50	2069,28
Valina	>50	2706,92

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citrato de sódio	12045026	20918	40	20120307
Caelo	Citrato de sódio	13089335	21670	60	AR-15-FG-000405-01

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citrato de sódio	14112517	21718	60	20140416
Euro OTC	Citrato de sódio	1506041	21839	60	0000010492
Euro OTC	Citrato de sódio	1511017	21997	60	20151130*
Euro OTC	Citrato de sódio	1610016	22859	40	20161102*
Euro OTC	Citrato de sódio	1701029	22996	40	20170126*
Euro OTC	Citrato de sódio	2007022	25324	40	20200820*
Fagron	Citrato de sódio	12E04-N05	20662	40	20120516
Fagron	Citrato de sódio	14A13-B02-294541	21778	60	20140424
Fagron	Citrato de sódio	16F10-B01-326088	22843	40	20160711

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 11 reference samples from the substance/substance group *Citrato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 152 422 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 810 spectra of 22 reference samples from the substance/substance group *Citrato de sódio*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citrato de sódio	162179	22618	40
Caelo	Citrato de sódio	173236	23789	40
Caelo	Citrato de sódio	182083	24218	40
Caelo	Citrato de sódio	190890	24533	40
Caelo	Citrato de sódio	20002150	25229	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citrato de sódio	22002778	26501	40
Euro OTC	Citrato de sódio	1604030	22510	40
Euro OTC	Citrato de sódio	1607040	22687	40
Euro OTC	Citrato de sódio	1710006	23614	40
Euro OTC	Citrato de sódio	1807035	24151	40
Euro OTC	Citrato de sódio	1901035	24487	40
Euro OTC	Citrato de sódio	1909020	24862	40
Euro OTC	Citrato de sódio	2002040	25127	40
Euro OTC	Citrato de sódio	2101007	25550	40
Euro OTC	Citrato de sódio	2206011	26221	40
Euro OTC	Citrato de sódio	2212001	26419	30
Euro OTC	Citrato de sódio	2307019	26862	40
Fagron	Citrato de sódio	22A15-B18-219203	26154	40
Fagron	Citrato de sódio	22K17-B15-223095	26983	40
Caelo	Citrato de sódio	22002778	26501SI	20
Euro OTC	Citrato de sódio	2206011	26221SI	20
Fagron	Citrato de sódio	22A15-B18-219203	26154SI	20

- 201 274 spectra from a total of 4026 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2248 spectra from 998 *Apo-Ident* customers from 423 batches from the substance/substance group *Citrato de sódio*.

- Among them are spectra of independent samples from 410 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citrato de sódio		1
	Citrato de sódio	1710006-01	1
	Citrato de sódio	18208302	1
	Citrato de sódio	190890007	1
	Citrato de sódio	21002580012	1
	Citrato de sódio	21002580018	1
	Citrato de sódio	21002580019	1
	Citrato de sódio	2101007-01	1
	Citrato de sódio	22002778001	1
	Citrato de sódio	22002778003	3
	Citrato de sódio	22002778007	17
	Citrato de sódio	22002778008	1
	Citrato de sódio	2212001-001	1
	Citrato de sódio	2212001-01	13
	Citrato de sódio	2212001-02	1
	Citrato de sódio	2212001-03	1
	Citrato de sódio	23000473002	11
	Citrato de sódio	23003487003	5
	Citrato de sódio	3118872	2
AHD	Citrato de sódio	1607040-01	2
AHD	Citrato de sódio	1710006-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Citrato de sódio	17323602	2
AHD	Citrato de sódio	1901035-01	1
AHD	Citrato de sódio	22002778003	1
Alli	Citrato de sódio	22002778007	1
Alliance Healthcare	Citrato de sódio	1211030-01	1
Alliance	Citrato de sódio	22002778003	1
Anzag	Citrato de sódio	1512705	1
Anzag	Citrato de sódio	20A20-F03-369331	1
Anzag	Citrato de sódio	21002580012	1
Anzag	Citrato de sódio	2212001-01	1
ApoIdent/ Phoenix	Citrato de sódio	1710006-01	1
apo-ident	Citrato de sódio	1701029-01	1
Apo-ident	Citrato de sódio	3065202	1
Audor Pharma	Citrato de sódio	171000601	1
Aug. Hedinger	Citrato de sódio	8765456	1
Bombastus	Citrato de sódio	73155098	1
Caelo	Citrato de sódio		15
Caelo	Citrato de sódio	1042	1
Caelo	Citrato de sódio	1107011-01	1
Caelo	Citrato de sódio	11081514	1
Caelo	Citrato de sódio	11121303	1
Caelo	Citrato de sódio	11219012	6
Caelo	Citrato de sódio	1123588946	1
Caelo	Citrato de sódio	11304311	3
Caelo	Citrato de sódio	1151351	2
Caelo	Citrato de sódio	1161207	2
Caelo	Citrato de sódio	1200002828764	1
Caelo	Citrato de sódio	12045001	1
Caelo	Citrato de sódio	12045002	1
Caelo	Citrato de sódio	12045004	4
Caelo	Citrato de sódio	12045006	1
Caelo	Citrato de sódio	12045008	4
Caelo	Citrato de sódio	12045011	6
Caelo	Citrato de sódio	12045012	1
Caelo	Citrato de sódio	12045016	5
Caelo	Citrato de sódio	12045016-3451311172	1
Caelo	Citrato de sódio	12045019	4
Caelo	Citrato de sódio	12045024	5
Caelo	Citrato de sódio	12045026	7
Caelo	Citrato de sódio	1223test	1
Caelo	Citrato de sódio	1234	3
Caelo	Citrato de sódio	123456	2
Caelo	Citrato de sódio	1234567	1
Caelo	Citrato de sódio	123456789	1
Caelo	Citrato de sódio	1234test	1
Caelo	Citrato de sódio	1234Test	3
Caelo	Citrato de sódio	12358Test	1
Caelo	Citrato de sódio	123658	1
Caelo	Citrato de sódio	123e2	1
Caelo	Citrato de sódio	123test	6
Caelo	Citrato de sódio	123Test	16
Caelo	Citrato de sódio	123tst	1
Caelo	Citrato de sódio	1256825	1
Caelo	Citrato de sódio	125874566	1
Caelo	Citrato de sódio	128896	1
Caelo	Citrato de sódio	12897	1
Caelo	Citrato de sódio	13/24-B13-287921	1
Caelo	Citrato de sódio	1308908	1
Caelo	Citrato de sódio	13089304	2
Caelo	Citrato de sódio	13089305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de sódio	13089308	7
Caelo	Citrato de sódio	13089314	1
Caelo	Citrato de sódio	13089317	7
Caelo	Citrato de sódio	13089319	4
Caelo	Citrato de sódio	13089325	3
Caelo	Citrato de sódio	13089329	1
Caelo	Citrato de sódio	13089331	5
Caelo	Citrato de sódio	13089335	8
Caelo	Citrato de sódio	131103501	1
Caelo	Citrato de sódio	1319A-01900	1
Caelo	Citrato de sódio	1404033-01	3
Caelo	Citrato de sódio	140510/1	1
Caelo	Citrato de sódio	140731NC	1
Caelo	Citrato de sódio	14112502	26
Caelo	Citrato de sódio	14112517	12
Caelo	Citrato de sódio	14112518	1
Caelo	Citrato de sódio	14112520	1
Caelo	Citrato de sódio	1411502	1
Caelo	Citrato de sódio	1412014-01	1
Caelo	Citrato de sódio	14360407	1
Caelo	Citrato de sódio	14369402	2
Caelo	Citrato de sódio	14369406	9
Caelo	Citrato de sódio	14369407	51
Caelo	Citrato de sódio	14369411	3
Caelo	Citrato de sódio	14369413	22
Caelo	Citrato de sódio	14369414	1
Caelo	Citrato de sódio	14369415	1
Caelo	Citrato de sódio	14369416	1
Caelo	Citrato de sódio	14369423	21
Caelo	Citrato de sódio	14369424	4
Caelo	Citrato de sódio	1469413	1
Caelo	Citrato de sódio	14838	1
Caelo	Citrato de sódio	14A13-B02_300395	1
Caelo	Citrato de sódio	1506041-01	1
Caelo	Citrato de sódio	151101701	1
Caelo	Citrato de sódio	1511017-01	3
Caelo	Citrato de sódio	15212705	5
Caelo	Citrato de sódio	154662	1
Caelo	Citrato de sódio	15C27-B01-309893	1
Caelo	Citrato de sódio	160704001	1
Caelo	Citrato de sódio	1607040-01	4
Caelo	Citrato de sódio	160955707	1
Caelo	Citrato de sódio	16095702	4
Caelo	Citrato de sódio	16095707	9
Caelo	Citrato de sódio	1610016-01	4
Caelo	Citrato de sódio	16217901	1
Caelo	Citrato de sódio	16217902	1
Caelo	Citrato de sódio	16217905	18
Caelo	Citrato de sódio	16217906	1
Caelo	Citrato de sódio	16217908	1
Caelo	Citrato de sódio	16217909	10
Caelo	Citrato de sódio	16217912	3
Caelo	Citrato de sódio	16217913	1
Caelo	Citrato de sódio	16217914	5
Caelo	Citrato de sódio	16217915	2
Caelo	Citrato de sódio	16F10-B01-326093	1
Caelo	Citrato de sódio	16F10-B01-327510	1
Caelo	Citrato de sódio	170102901	1
Caelo	Citrato de sódio	1701029-01	5
Caelo	Citrato de sódio	17081501	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de sódio	1710006-02	1
Caelo	Citrato de sódio	171006-02	1
Caelo	Citrato de sódio	171025NC/16217909	1
Caelo	Citrato de sódio	17323601	34
Caelo	Citrato de sódio	17323602	7
Caelo	Citrato de sódio	17323603	6
Caelo	Citrato de sódio	17323608	39
Caelo	Citrato de sódio	17323609	8
Caelo	Citrato de sódio	1732361	1
Caelo	Citrato de sódio	17323612	5
Caelo	Citrato de sódio	1732601	1
Caelo	Citrato de sódio	1732608	1
Caelo	Citrato de sódio	1792380	1
Caelo	Citrato de sódio	17H7-B04-345098	1
Caelo	Citrato de sódio	18028305	1
Caelo	Citrato de sódio	1807035-01	2
Caelo	Citrato de sódio	1807035-02	2
Caelo	Citrato de sódio	1807053-01	1
Caelo	Citrato de sódio	18208302	22
Caelo	Citrato de sódio	18208303	8
Caelo	Citrato de sódio	18208305	1
Caelo	Citrato de sódio	18208307	23
Caelo	Citrato de sódio	18208308	4
Caelo	Citrato de sódio	18208313	8
Caelo	Citrato de sódio	18208314	3
Caelo	Citrato de sódio	18208315	32
Caelo	Citrato de sódio	18G25-B07-352737	1
Caelo	Citrato de sódio	1901035-01	3
Caelo	Citrato de sódio	190890002	11
Caelo	Citrato de sódio	190890003	2
Caelo	Citrato de sódio	190890004	3
Caelo	Citrato de sódio	190890005	3
Caelo	Citrato de sódio	190890007	19
Caelo	Citrato de sódio	190890009	28
Caelo	Citrato de sódio	19089001	4
Caelo	Citrato de sódio	19089002	6
Caelo	Citrato de sódio	19089003	11
Caelo	Citrato de sódio	19089004	30
Caelo	Citrato de sódio	1909020-01	1
Caelo	Citrato de sódio	19121802	1
Caelo	Citrato de sódio	20002150001	2
Caelo	Citrato de sódio	20002150003	4
Caelo	Citrato de sódio	20004144004	1
Caelo	Citrato de sódio	20004144005	3
Caelo	Citrato de sódio	20004144008	1
Caelo	Citrato de sódio	20004144010	1
Caelo	Citrato de sódio	2016-01-28AVIGr	1
Caelo	Citrato de sódio	20170412	1
Caelo	Citrato de sódio	2019Q-01900	1
Caelo	Citrato de sódio	21002580003	4
Caelo	Citrato de sódio	21002580004	6
Caelo	Citrato de sódio	21002580007	4
Caelo	Citrato de sódio	21002580008	2
Caelo	Citrato de sódio	21002580009	2
Caelo	Citrato de sódio	21002580010	2
Caelo	Citrato de sódio	21002580011	2
Caelo	Citrato de sódio	21002580012	12
Caelo	Citrato de sódio	21002580013	1
Caelo	Citrato de sódio	21002580015	1
Caelo	Citrato de sódio	21002580016	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato de sódio	21002580018	5
Caelo	Citrato de sódio	21002580019	1
Caelo	Citrato de sódio	2101007-01	3
Caelo	Citrato de sódio	21121203	1
Caelo	Citrato de sódio	2116A-01900	1
Caelo	Citrato de sódio	22002778002	1
Caelo	Citrato de sódio	22002778003	6
Caelo	Citrato de sódio	22002778007	8
Caelo	Citrato de sódio	220516(190890009)	1
Caelo	Citrato de sódio	220914PML01	1
Caelo	Citrato de sódio	23003487003	1
Caelo	Citrato de sódio	2345678	1
Caelo	Citrato de sódio	2413A-01900	1
Caelo	Citrato de sódio	25383143	1
Caelo	Citrato de sódio	2543	1
Caelo	Citrato de sódio	2815A-01900	1
Caelo	Citrato de sódio	2818A-01900	1
Caelo	Citrato de sódio	2908022-01	1
Caelo	Citrato de sódio	30081802	1
Caelo	Citrato de sódio	3040611	1
Caelo	Citrato de sódio	4111Q-01900	1
Caelo	Citrato de sódio	459842	1
Caelo	Citrato de sódio	4680	1
Caelo	Citrato de sódio	49131-01900	1
Caelo	Citrato de sódio	50815PMS01	1
Caelo	Citrato de sódio	516-01900	1
Caelo	Citrato de sódio	70214PJK01	1
Caelo	Citrato de sódio	8/AKD41	1
Caelo	Citrato de sódio	AM1007248703	1
Caelo	Citrato de sódio	K-280313-1	1
Caelo	Citrato de sódio	P-07081921/18208313	1
Caelo	Citrato de sódio	Test	3
Caelo	Citrato de sódio	Test123	1
Caelo	Citrato de sódio	test13	1
Caelo	Citrato de sódio	Testmessung	1
Caelo	Citrato de sódio	TestmessungnachRep	1
Caelo	Citrato de sódio	Validierungsmessung	1
caeo	Citrato de sódio	22002778003	1
Caesar & Loretz / Sa…	Citrato de sódio	190890007	1
Caesar & Loretz GmbH…	Citrato de sódio	14369406	1
Caesar & Loretz GmbH…	Citrato de sódio	20004144005	1
Caesar & Loretz GmbH…	Citrato de sódio	21002580003	1
Caesar & Loretz GmbH…	Citrato de sódio	18208302	2
Caesar & Loretz GmbH…	Citrato de sódio	20002150001	1
Caesar & Loretz GmbH…	Citrato de sódio	190890002	1
Caesar & Loretz GmbH /AHD	Citrato de sódio	22002778007	1
Caesar & Loretz GmbH/ AHD	Citrato de sódio	18208315	1
Caesar & Loretz GmbH…	Citrato de sódio	190890007	1
Caesar & Loretz GmbH…	Citrato de sódio	19089003	1
Caesar & Loretz GmbH/Gehe	Citrato de sódio	18208302	1
Caesar & Loretz GmbH/Gehe	Citrato de sódio	18208315	1
Caesar & Loretz GmbH/Gehe	Citrato de sódio	21002580003	1
Caesar & Loretz GmbH…	Citrato de sódio	190890009	1
Caesar & Loretz GmbH/K	Citrato de sódio	190890009	1
Caesar & Loretz GmbH…	Citrato de sódio	18208307	1
Caesar & Loretz GmbH…	Citrato de sódio	190890009	1
Caesar & Loretz GmbH…	Citrato de sódio	19089004	2
Caesar & Loretz GmbH…	Citrato de sódio	19089002	1
Caesar & Loretz GmbH…	Citrato de sódio	22002778003	1
Caesar & Loretz GmbH…	Citrato de sódio	1701029-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Citrato de sódio	18208315	2
Caesar & Loretz GmbH...	Citrato de sódio	190890009	1
Caesar & Loretz GmbH...	Citrato de sódio	19089004	2
Caesar & Loretz GmbH	Citrato de sódio	13089334	1
Caesar & Loretz GmbH	Citrato de sódio	14112517	1
Caesar & Loretz GmbH	Citrato de sódio	14369406	1
Caesar & Loretz GmbH	Citrato de sódio	1607040-01	1
Caesar & Loretz GmbH	Citrato de sódio	17323601	1
Caesar & Loretz GmbH	Citrato de sódio	17323608	1
Caesar & Loretz GmbH	Citrato de sódio	18208302	4
Caesar & Loretz GmbH	Citrato de sódio	18208305	1
Caesar & Loretz GmbH	Citrato de sódio	18208307	4
Caesar & Loretz GmbH	Citrato de sódio	18208308	1
Caesar & Loretz GmbH	Citrato de sódio	18208315	5
Caesar & Loretz GmbH	Citrato de sódio	190890002	3
Caesar & Loretz GmbH	Citrato de sódio	190890003	3
Caesar & Loretz GmbH	Citrato de sódio	190890004	4
Caesar & Loretz GmbH	Citrato de sódio	190890007	8
Caesar & Loretz GmbH	Citrato de sódio	190890009	9
Caesar & Loretz GmbH	Citrato de sódio	19089002	2
Caesar & Loretz GmbH	Citrato de sódio	19089003	3
Caesar & Loretz GmbH	Citrato de sódio	19089004	7
Caesar & Loretz GmbH	Citrato de sódio	1909020-01	1
Caesar & Loretz GmbH	Citrato de sódio	20002150003	4
Caesar & Loretz GmbH	Citrato de sódio	21002580004	1
Caesar & Loretz GmbH	Citrato de sódio	21002580007	1
Caesar & Loretz GmbH	Citrato de sódio	21002580009	2
Caesar & Loretz GmbH	Citrato de sódio	2100258001	1
Caesar & Loretz GmbH	Citrato de sódio	21002580010	1
Caesar & Loretz GmbH	Citrato de sódio	21002580011	3
Caesar & Loretz GmbH	Citrato de sódio	21002580012	3
Caesar & Loretz GmbH	Citrato de sódio	22002778003	1
Caesar & Loretz/Geil...	Citrato de sódio	190890007	1
Caesar&Loretz GmbH/Anzag	Citrato de sódio	14369407	1
Caesar&Loretz GmbH	Citrato de sódio	12045026	1
Caesar&Loretz GmbH	Citrato de sódio	14112502	1
Caesar/Noweda	Citrato de sódio	12045008	1
Caeser und Loretz GmbH	Citrato de sódio	18208308	1
Caleo	Citrato de sódio	18208302	1
Calo, Hilden/ Phönix	Citrato de sódio	19089004	1
Cealo/Sanacorp	Citrato de sódio	21002580012	1
Cealo	Citrato de sódio	190890007	1
Defektur	Citrato de sódio	19121902	1
Delta Apotheke	Citrato de sódio	17323608	1
Eigenherstellung Defektur	Citrato de sódio	5082103	1
Eigenherstellung/ De...	Citrato de sódio	12102101	1
EuRho / Alliance	Citrato de sódio	1807035-02	1
EuRho / Noweda	Citrato de sódio	1807035-01	1
EuRho / Phoenix	Citrato de sódio	151101017-01	1
EuRho/ AHD	Citrato de sódio	1701029-01	1
EuRho/ Phönix	Citrato de sódio	3048768	1
EuRho/Gehe	Citrato de sódio	1901035-01	2
EuRho/Jenne	Citrato de sódio	1909020-01	1
EuRho/Noweda	Citrato de sódio	2206011-01	1
EuRho/Sanacorp	Citrato de sódio	1107011-02	1
EuRho/Sanacorp	Citrato de sódio	1506041-01	1
EuRho	Citrato de sódio	1070102901	1
EuRho	Citrato de sódio	1107011-02	1
EuRho	Citrato de sódio	1205026-02	1
EuRho	Citrato de sódio	1211030-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Citrato de sódio	1311035-01	1
EuRho	Citrato de sódio	140403301	1
EuRho	Citrato de sódio	1404033-01	2
EuRho	Citrato de sódio	1412014-01	1
EuRho	Citrato de sódio	1607040-01	5
EuRho	Citrato de sódio	1901035-01	1
Eurho	Citrato de sódio	2007022-01	1
EuRho	Citrato de sódio	2007022-01	1
Eurho	Citrato de sódio	2101007-01	1
EuRho	Citrato de sódio	3032981	1
EuRho	Citrato de sódio	3108854	1
EuRho	Citrato de sódio	4611M-01900	1
Euro Gehe	Citrato de sódio	1909020-01	1
Euro OTC	Citrato de sódio		5
Euro OTC	Citrato de sódio	100800903	1
Euro OTC	Citrato de sódio	1017I-01900	1
Euro OTC	Citrato de sódio	1073240	1
Euro OTC	Citrato de sódio	1107011-01	1
Euro OTC	Citrato de sódio	1107011-02	1
Euro OTC	Citrato de sódio	1205026-02	4
Euro OTC	Citrato de sódio	1211030-01	10
Euro OTC	Citrato de sódio	12345	2
Euro OTC	Citrato de sódio	1305001-01	11
Euro OTC	Citrato de sódio	1311025-01	1
Euro OTC	Citrato de sódio	1311035-01	27
Euro OTC	Citrato de sódio	13I24-B13-287921	1
Euro OTC	Citrato de sódio	140403301	5
Euro OTC	Citrato de sódio	1404033-01	13
Euro OTC	Citrato de sódio	1412014-01	18
Euro OTC	Citrato de sódio	1413M-01900	1
Euro OTC	Citrato de sódio	14201401	1
Euro OTC	Citrato de sódio	1506041-01	18
Euro OTC	Citrato de sódio	150922-1078	1
Euro OTC	Citrato de sódio	151101701	3
Euro OTC	Citrato de sódio	1511017-01	32
Euro OTC	Citrato de sódio	15111017-01	1
Euro OTC	Citrato de sódio	1521017-01	1
Euro OTC	Citrato de sódio	15212705	1
Euro OTC	Citrato de sódio	156422	1
Euro OTC	Citrato de sódio	16070-01	1
Euro OTC	Citrato de sódio	1607040-01	20
Euro OTC	Citrato de sódio	160740-01	1
Euro OTC	Citrato de sódio	161001601	1
Euro OTC	Citrato de sódio	1610016-01	45
Euro OTC	Citrato de sódio	1610016601	1
Euro OTC	Citrato de sódio	1645265	3
Euro OTC	Citrato de sódio	17010006-02	1
Euro OTC	Citrato de sódio	170102901	1
Euro OTC	Citrato de sódio	1701029-01	43
Euro OTC	Citrato de sódio	1701029-02	1
Euro OTC	Citrato de sódio	17061407	1
Euro OTC	Citrato de sódio	1710006-01	12
Euro OTC	Citrato de sódio	1710006-015607	1
Euro OTC	Citrato de sódio	1710006-02	10
Euro OTC	Citrato de sódio	171006-02	1
Euro OTC	Citrato de sódio	180703501	1
Euro OTC	Citrato de sódio	1807035-01	36
Euro OTC	Citrato de sódio	1807035-01ciclo	1
Euro OTC	Citrato de sódio	1807035-02	10
Euro OTC	Citrato de sódio	180735-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Citrato de sódio	1819A-01900	1
Euro OTC	Citrato de sódio	187035-01	1
Euro OTC	Citrato de sódio	19009020-01	1
Euro OTC	Citrato de sódio	190103501	1
Euro OTC	Citrato de sódio	1901035-01	52
Euro OTC	Citrato de sódio	19090120-01	1
Euro OTC	Citrato de sódio	1909020	1
Euro OTC	Citrato de sódio	1909020-01	38
Euro OTC	Citrato de sódio	190902-01	1
Euro OTC	Citrato de sódio	190920	1
Euro OTC	Citrato de sódio	2002040-01	30
Euro OTC	Citrato de sódio	2002040-1	1
Euro OTC	Citrato de sódio	200702201	1
Euro OTC	Citrato de sódio	2007022-01	37
Euro OTC	Citrato de sódio	20200810-6	1
Euro OTC	Citrato de sódio	20A20-FO3-369331	1
Euro OTC	Citrato de sódio	2101007	2
Euro OTC	Citrato de sódio	210100701	1
Euro OTC	Citrato de sódio	2101007-01	44
Euro OTC	Citrato de sódio	2114M1900	1
Euro OTC	Citrato de sódio	2206011-01	30
Euro OTC	Citrato de sódio	22101305	1
Euro OTC	Citrato de sódio	2212001-01	1
Euro OTC	Citrato de sódio	22606011-01	1
Euro OTC	Citrato de sódio	23062015C	1
Euro OTC	Citrato de sódio	25425	2
Euro OTC	Citrato de sódio	2546426	1
Euro OTC	Citrato de sódio	2903001-01	1
Euro OTC	Citrato de sódio	30111301	1
Euro OTC	Citrato de sódio	3021717	1
Euro OTC	Citrato de sódio	3032805	3
Euro OTC	Citrato de sódio	3032981	1
Euro OTC	Citrato de sódio	3048768	3
Euro OTC	Citrato de sódio	30611044	5
Euro OTC	Citrato de sódio	3065202	2
Euro OTC	Citrato de sódio	3087522	2
Euro OTC	Citrato de sódio	3095222	3
Euro OTC	Citrato de sódio	3108854	1
Euro OTC	Citrato de sódio	3454	1
Euro OTC	Citrato de sódio	345678	1
Euro OTC	Citrato de sódio	358528	1
Euro OTC	Citrato de sódio	4716E-01900	1
Euro OTC	Citrato de sódio	48(08598497)	1
Euro OTC	Citrato de sódio	5116E-01900	1
Euro OTC	Citrato de sódio	815757/6745	1
Euro OTC	Citrato de sódio	901035-011	1
euro//Noweda	Citrato de sódio	1701029-01	1
Euro/Phönix	Citrato de sódio	1305001-01	1
Euro/Phönix	Citrato de sódio	1610016-01	1
Euro	Citrato de sódio	1815M-01900	1
Europ Ots Pharma	Citrato de sódio	13089304	1
Fagron	Citrato de sódio	1017Q-01900	1
Fagron	Citrato de sódio	1161207	3
Fagron	Citrato de sódio	1172108	1
Fagron	Citrato de sódio	1176767	3
Fagron	Citrato de sódio	1190802	1
Fagron	Citrato de sódio	1211142	2
Fagron	Citrato de sódio	1219546	2
Fagron	Citrato de sódio	1227297	3
Fagron	Citrato de sódio	1232850	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Citrato de sódio	12339502	1
Fagron	Citrato de sódio	1234468	1
Fagron	Citrato de sódio	1234567	1
Fagron	Citrato de sódio	123456test	1
Fagron	Citrato de sódio	1241068	1
Fagron	Citrato de sódio	1250221	2
Fagron	Citrato de sódio	1262240	4
Fagron	Citrato de sódio	12A05-N04	2
Fagron	Citrato de sódio	12E04-N05	1
Fagron	Citrato de sódio	12I10-N01	1
Fagron	Citrato de sódio	12J26-N02	3
Fagron	Citrato de sódio	13/24-B13-287921	3
Fagron	Citrato de sódio	13089331	1
Fagron	Citrato de sódio	13A07-N01	6
Fagron	Citrato de sódio	13A07-NO1	1
Fagron	Citrato de sódio	13B28-N02	6
Fagron	Citrato de sódio	13D09N01	1
Fagron	Citrato de sódio	13D09-N01	4
Fagron	Citrato de sódio	13I24-B13-287921	2
Fagron	Citrato de sódio	13l24-B13	1
Fagron	Citrato de sódio	14112502	2
Fagron	Citrato de sódio	14369402	2
Fagron	Citrato de sódio	14A13_b02_300395	1
Fagron	Citrato de sódio	14A13-B02-294541	8
Fagron	Citrato de sódio	14A13B02300395	1
Fagron	Citrato de sódio	14A13-B02-300395	4
Fagron	Citrato de sódio	1511017-01	1
Fagron	Citrato de sódio	15C27	1
Fagron	Citrato de sódio	15C27-B01-309893	5
Fagron	Citrato de sódio	15-C27-B01-309893	1
Fagron	Citrato de sódio	15C27-B01-312231	6
Fagron	Citrato de sódio	15C27-B01-316106	2
Fagron	Citrato de sódio	15c27-b01-321097	1
Fagron	Citrato de sódio	15C27B01-321097	1
Fagron	Citrato de sódio	15C27-B01-321097	1
Fagron	Citrato de sódio	15C27-B01-3211097	1
Fagron	Citrato de sódio	15C27-B01-323451	3
Fagron	Citrato de sódio	15C27-B01-3234551	1
Fagron	Citrato de sódio	160614	1
Fagron	Citrato de sódio	16217912	2
Fagron	Citrato de sódio	16F10-B01-326088	2
Fagron	Citrato de sódio	16F10-B01-327510	5
Fagron	Citrato de sódio	16F10-B1-327510	1
Fagron	Citrato de sódio	1710006-01	1
Fagron	Citrato de sódio	179915	3
Fagron	Citrato de sódio	179915-0001	2
Fagron	Citrato de sódio	17A26-B04-331525	1
Fagron	Citrato de sódio	17A26-B04-331528	14
Fagron	Citrato de sódio	17A26-B04-332866	1
Fagron	Citrato de sódio	17A26-B04-332871	26
Fagron	Citrato de sódio	17A26-B04-335680	24
Fagron	Citrato de sódio	17A26-B04-335883	2
Fagron	Citrato de sódio	17H04-B04-345098	1
Fagron	Citrato de sódio	17H07	1
Fagron	Citrato de sódio	17H07-B04	2
Fagron	Citrato de sódio	17H07-B04_338530	28
Fagron	Citrato de sódio	17H07-B04-341746	5
Fagron	Citrato de sódio	17H07-B04-345098	2
Fagron	Citrato de sódio	1807035-01	1
Fagron	Citrato de sódio	18B14-B08	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Citrato de sódio	18B14-B08-348067	6
Fagron	Citrato de sódio	18C05-B03	2
Fagron	Citrato de sódio	18C05-B03350564	1
Fagron	Citrato de sódio	18C05-B03-350564	3
Fagron	Citrato de sódio	18G25-B07	2
Fagron	Citrato de sódio	18G25-B07-352737	4
Fagron	Citrato de sódio	18G25-B07-354623	2
Fagron	Citrato de sódio	18G25-B07-354812	4
Fagron	Citrato de sódio	18L13B023549449	1
Fagron	Citrato de sódio	18l13b02359449	1
Fagron	Citrato de sódio	18L13-B02-359449	11
Fagron	Citrato de sódio	18L13-B02-359451	3
Fagron	Citrato de sódio	18L13-Bo2-359449	1
Fagron	Citrato de sódio	18L13-BO2-359449	1
Fagron	Citrato de sódio	19F19-B01	2
Fagron	Citrato de sódio	19F19-B01-363699	2
Fagron	Citrato de sódio	19F19-B01-363701	4
Fagron	Citrato de sódio	19I26-F01-365434	4
Fagron	Citrato de sódio	19I26F01365444	1
Fagron	Citrato de sódio	19I26FO1365444	1
Fagron	Citrato de sódio	19l26-F01-365434	1
Fagron	Citrato de sódio	2007022-01	1
Fagron	Citrato de sódio	20A20F03	1
Fagron	Citrato de sódio	20A20-F03	4
Fagron	Citrato de sódio	20A20-F03-069331	1
Fagron	Citrato de sódio	20A20-f03-368130	1
Fagron	Citrato de sódio	20A20-F03-368130	11
Fagron	Citrato de sódio	20A20-F03-369331	5
Fagron	Citrato de sódio	20A20-F03-369333	13
Fagron	Citrato de sódio	20B24-F03-374173	1
Fagron	Citrato de sódio	20K19-F02	1
Fagron	Citrato de sódio	20K19-F02-376135	1
Fagron	Citrato de sódio	20K19-F02-376136	2
Fagron	Citrato de sódio	22K17-B15-221097	1
Fagron	Citrato de sódio	22K17-B15-22197	1
Fagron	Citrato de sódio	2412130l	1
Fagron	Citrato de sódio	2OA2O-FO3-368130	1
Fagron	Citrato de sódio	2OA2O-FO3-369331	1
Fagron	Citrato de sódio	2OAO-FO3-368130	1
Fagron	Citrato de sódio	2OB24-FO3374173	1
Fagron	Citrato de sódio	306084	1
Fagron	Citrato de sódio	31051202	1
Fagron	Citrato de sódio	3311E-01900	1
Fagron	Citrato de sódio	712A-01900	1
Fagron	Citrato de sódio	801-3636909	1
Fagron	Citrato de sódio	815Q-01900	1
Fagron	Citrato de sódio	F03-368130	1
Fagron	Citrato de sódio	F03-3681300	1
Fagron	Citrato de sódio	F0336813000	1
Fagron	Citrato de sódio	F03-3693301	1
Fagron	Citrato de sódio	Probe	1
Fargo/Phoenix	Citrato de sódio	1511017-01	1
Fargon GmbH & Co.KG	Citrato de sódio	16F10-B01-326088	1
Fargon/Alliance HC	Citrato de sódio	13/24-B13-287921	1
fargon	Citrato de sódio	100772-114-91	1
Fiebig	Citrato de sódio	12J26-NO2	1
Fiebig	Citrato de sódio	1607002-01	2
Fiebig	Citrato de sódio	1610016-01	1
Fiebig	Citrato de sódio	190890002	1
Fragon	Citrato de sódio	18L13-BO2-359449	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gatt-Koller	Citrato de sódio	1073/04121412	1
Gehe 26.05.2014	Citrato de sódio	13B28-N02	1
Gehe amax	Citrato de sódio	1610016-01	1
Gehe Rostock	Citrato de sódio	2002040-01	1
Gehe/Euro	Citrato de sódio	1404033-01	2
Gehe/Euro	Citrato de sódio	1412014-01	6
Gehe	Citrato de sódio	12045026	1
Gehe	Citrato de sódio	1311035-01	1
Gehe	Citrato de sódio	14369413	2
GEHE	Citrato de sódio	1710006-02	1
GEHE	Citrato de sódio	17A26-B04-331525	6
GEHE	Citrato de sódio	17A26-B04-332866	5
GEHE	Citrato de sódio	17H507-A04-347340	1
Gehe	Citrato de sódio	18B14-B08-348067	1
Gehe	Citrato de sódio	18G25-B07	1
gehe	Citrato de sódio	18G25-B07-354812	1
Gehe	Citrato de sódio	18L13-B02-359449	1
Gehe	Citrato de sódio	1901035-01	3
Gehe	Citrato de sódio	19089003	1
Gehe	Citrato de sódio	2007022-01	1
GEHE	Citrato de sódio	21002580016	1
Gehe	Citrato de sódio	2101007-01	1
Gehe	Citrato de sódio	22002778007	2
Gehe	Citrato de sódio	2206011-01	1
Gehe	Citrato de sódio	2212001-01	2
GEHE	Citrato de sódio	2212001-01	1
Hageda	Citrato de sódio	2002040-01	1
HiperScan	Citrato de sódio		1
Jenne	Citrato de sódio	21002580007	1
Jungbunzlauer/Phoenix	Citrato de sódio	20A20-F03	1
Kehr	Citrato de sódio	17A26-B04-331525	1
Kehr	Citrato de sódio	23000473002	1
L12	Citrato de sódio	16217905	1
L12	Citrato de sódio	17323608	1
Merck	Citrato de sódio		2
Merck	Citrato de sódio	37/17	1
Merck	Citrato de sódio	AM0602648542	1
Merck	Citrato de sódio	AM1005848809	1
Merck	Citrato de sódio	AM1171048839	1
Merck	Citrato de sódio	AM1171148726	1
Merk	Citrato de sódio	AM0602648	1
Nachprüfung 31.12.2018	Citrato de sódio	14112517	2
Nachprüfung	Citrato de sódio	1205026-02	1
Noweda	Citrato de sódio	11127001	1
Noweda	Citrato de sódio	12045026	1
Noweda	Citrato de sódio	14A13-B02-294541	1
Noweda	Citrato de sódio	1511017-01	1
Noweda	Citrato de sódio	16095707	1
Noweda	Citrato de sódio	1701029-01	1
Noweda	Citrato de sódio	1710006-01	1
Noweda	Citrato de sódio	17H07-B04	1
Noweda	Citrato de sódio	17H07-B04-341746	1
Noweda	Citrato de sódio	17H07-B04-345098	1
Noweda	Citrato de sódio	18208315	2
Noweda	Citrato de sódio	1901035-01	1
Noweda	Citrato de sódio	1909020-01	1
Noweda	Citrato de sódio	19F19-B01-363699	1
Noweda	Citrato de sódio	22002778007	3
Noweda	Citrato de sódio	2202778003	1
Noweda	Citrato de sódio	2212001-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Citrato de sódio	22K17-B15-221097	1
Noweda	Citrato de sódio	3032981	1
Nowedan 15.11.2019	Citrato de sódio	1909020-01	1
Phoenix /Fargon	Citrato de sódio	20A20-F03-368130	1
Phoenix 30.05.2016	Citrato de sódio	14369423	1
Phoenix/Noweda	Citrato de sódio	1506041-01	2
Phoenix	Citrato de sódio	1506041-01	1
Phoenix	Citrato de sódio	1511017-01	2
Phoenix	Citrato de sódio	1710006-02	1
Phoenix	Citrato de sódio	1901035-01	2
Phoenix	Citrato de sódio	191291911	1
Phoenix	Citrato de sódio	20a20-f03-368130	1
Phoenix	Citrato de sódio	22002778007	1
Phoenix	Citrato de sódio	2212001-01	1
Phoenix	Citrato de sódio	3422	1
Phönix	Citrato de sódio	12045019	1
Phönix	Citrato de sódio	12045024	1
Phönix	Citrato de sódio	1205026-02	1
Phönix	Citrato de sódio	1807035-01	2
Phönix	Citrato de sódio	1807035-02	1
Phönix	Citrato de sódio	190890007	1
Phönix	Citrato de sódio	21002580012	1
Phönix	Citrato de sódio	22002778003	3
Phönix	Citrato de sódio	22002778007	2
Phönix	Citrato de sódio	22K17-B15-223095	1
Retest	Citrato de sódio	1610016-01	1
Röntgen	Citrato de sódio	17323601	1
Sanacoro W.E:15.05.1…	Citrato de sódio	14112502	1
Sanacorp	Citrato de sódio	13089308	1
Sanacorp	Citrato de sódio	13089331	1
Sanacorp	Citrato de sódio	1311035-01	1
Sanacorp	Citrato de sódio	1436407	1
Sanacorp	Citrato de sódio	17A26-B04-332866	1
Sanacorp	Citrato de sódio	190890007	1
Sanacorp	Citrato de sódio	21002580012	1
Sanacorp	Citrato de sódio	21002580013	1
Sanacorp	Citrato de sódio	2101007-01	1
Sanacorp	Citrato de sódio	22002778007	1
Sanacorp	Citrato de sódio	2206011-01	1
Sanacorp	Citrato de sódio	2212001-01	1
Sanacorp	Citrato de sódio	23003487003	1
Sanacorp	Citrato de sódio	EuRho	1
Test	Citrato de sódio		1
TEST	Citrato de sódio		1
Test	Citrato de sódio	1234	1
Test	Citrato de sódio	12345	1
Test	Citrato de sódio	123456	1
Unisan	Citrato de sódio	1701029-01	1
Unisan	Citrato de sódio	S/WReferenzUmstell	1
VDL;16.05.15;3,83EUR	Citrato de sódio	14369406	1
wepa	Citrato de sódio	1909020-01	1

- 233 819 spectra from 1513 *Apo-Ident* customers from a total of 48 855 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	810	0	201 274
Type C	0	2120	128	233 819

The substance/substance group *Citrato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2593 %)
Type C	100.0000 % (> 99.9007 %)	94.3060 % (> 94.1726 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20662	21839	6,84	137,95
20918	21670	8,62	138,21
21670	21670	0,00	136,73
21718	21670	4,04	135,97
21778	21670	5,55	137,64
21839	21839	0,00	139,28
21997	21997	0,00	140,14
22843	21997	9,04	143,22
22859	22859	0,00	147,85
22996	22996	0,00	140,40
25324	25324	0,00	143,35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrato monobásico de magnésio, hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20016-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrato monobásico de magnésio, hidratado; Magnesii hydrogenocitras hydricus

Special notes

When selecting the *Citrato monobásico de magnésio, hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrato monobásico de magnésio, hidratado	11	34	251

Second-stage model

For differentiation of the substance/substance group *Citrato monobásico de magnésio, hidratado* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrato monobásico de magnésio, hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	48,65	–
Fosfato sódico de riboflavina hidratado	62,79	–
⋮	⋮	⋮
Sulfato de atropina	>50	76,24
Escina, hidrossolúvel	>50	92,51
Furoato de mometasona	>50	124,80
Orotato de cálcio di-hidratado	>50	157,33
Quinolina amarela	>50	161,83
Sacarina sódica	>50	177,51
Hidrocortisona	>50	198,83
Cloridrato de propranolol	>50	319,89
Sorbato de potássio	>50	479,19
Fenitoína	>50	584,28

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrato monobásico de magnésio, hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrato monobásico de magnésio, hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citrato monobásico de mag…	13389102	21445	60	20131205
Caelo	Citrato monobásico de mag…	15415014	23240	40	20160105
Caelo	Citrato monobásico de mag…	22001882	26251	40	2211127
Euro OTC	Citrato monobásico de mag…	1507010	21873	60	20150713*
Euro OTC	Citrato monobásico de mag…	1510033	22233	60	20151117*
Euro OTC	Citrato monobásico de mag…	1601005	22296	60	20160119*
Euro OTC	Citrato monobásico de mag…	1701003	22992	40	20170124*
Euro OTC	Citrato monobásico de mag…	2101004	25545	40	20210114*
Euro OTC	Citrato monobásico de mag…	2211017	26423	40	20221213*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Gatt-Koller	Citrato monobásico de mag…	22J01469	26400	40	2301186
Gatt-Koller	Citrato monobásico de mag…	22J01469	26400SI	20	2301186
Gatt-Koller	Citrato monobásico de mag…	24J00867	27302	40	20240620

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 12 reference samples from the substance/substance group *Citrato monobásico de magnésio, hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 422 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1490 spectra of 40 reference samples from the substance/substance group *Citrato monobásico de magnésio, hidratado*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citrato monobásico de mag…	173531	23788	40
Caelo	Citrato monobásico de mag…	182746	24397	40
Caelo	Citrato monobásico de mag…	21000135	25694	50
Caelo	Citrato monobásico de mag…	23001929	26956	40
Caelo	Citrato monobásico de mag…	24000609	27126	40
Caelo	Citrato monobásico de mag…	24001460	27305	40
Euro OTC	Citrato monobásico de mag…	1604002	22509	40
Euro OTC	Citrato monobásico de mag…	1608004	22796	40
Euro OTC	Citrato monobásico de mag…	1701004	22991	40
Euro OTC	Citrato monobásico de mag…	1705010	23380	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Citrato monobásico de mag…	1705009	23382	40
Euro OTC	Citrato monobásico de mag…	1710007	23771	40
Euro OTC	Citrato monobásico de mag…	1802026	24064	40
Euro OTC	Citrato monobásico de mag…	1811038	24425	40
Euro OTC	Citrato monobásico de mag…	1904011	24620	40
Euro OTC	Citrato monobásico de mag…	1907020	24777	40
Euro OTC	Citrato monobásico de mag…	1910005	24934	40
Euro OTC	Citrato monobásico de mag…	2003064	25261	40
Euro OTC	Citrato monobásico de mag…	2005027	25281	40
Euro OTC	Citrato monobásico de mag…	2009007	25329	40
Euro OTC	Citrato monobásico de mag…	2104021	25679	40
Euro OTC	Citrato monobásico de mag…	2107008	25777	50
Euro OTC	Citrato monobásico de mag…	2110009	25871	50
Euro OTC	Citrato monobásico de mag…	2201004	25918	40
Euro OTC	Citrato monobásico de mag…	2206017	26202	40
Euro OTC	Citrato monobásico de mag…	2304016	26644	40
Euro OTC	Citrato monobásico de mag…	2303006	26648	40
Euro OTC	Citrato monobásico de mag…	2307001	26878	40
Euro OTC	Citrato monobásico de mag…	2310019	26999	40
Euro OTC	Citrato monobásico de mag…	2403003	27195	40
Euro OTC	Citrato monobásico de mag…	2407003	27348	40
Fagron	Citrato monobásico de mag…	19I23-B02-195296	24953	40
Fagron	Citrato monobásico de mag…	22F02-B17-221504	26170	40
Gatt-Koller	Citrato monobásico de mag…	22J00225	26399	40
Caelo	Citrato monobásico de mag…	22001882	26251SI[†]	20
Euro OTC	Citrato monobásico de mag…	2110009	25871SI	10
Euro OTC	Citrato monobásico de mag…	2201004	25918SI	10
Euro OTC	Citrato monobásico de mag…	2206017	26202SI	20
Fagron	Citrato monobásico de mag…	22F02-B17-221504	26170SI	20
Gatt-Koller	Citrato monobásico de mag…	22J00225	26399SI	20

- 200 594 spectra from a total of 4010 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 811 spectra from 282 *Apo-Ident* customers from 256 batches from the substance/substance group *Citrato monobásico de magnésio, hidratado*.

- Among them are spectra of independent samples from 249 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citrato monobásico de mag…	1311003-01	1
	Citrato monobásico de mag…	1510033-01	1
	Citrato monobásico de mag…	22001882002	1
	Citrato monobásico de mag…	22001882003	1
	Citrato monobásico de mag…	22002876002	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Citrato monobásico de mag…	23001929001	1
	Citrato monobásico de mag…	23002924003	1
	Citrato monobásico de mag…	2304016-01	1
	Citrato monobásico de mag…	24001460001	1
/Sanacorp	Citrato monobásico de mag…	90170	1
ACM	Citrato monobásico de mag…	KNC0829J15	1
ACM	Citrato monobásico de mag…	KNC1377J15	2
AHD	Citrato monobásico de mag…	13389103	1
Alliance health	Citrato monobásico de mag…	13389111	2
Alliance	Citrato monobásico de mag…	181103801	1
Anzag	Citrato monobásico de mag…	16341710	1
AppliChem	Citrato monobásico de mag…	7V008966	1
Bombastus	Citrato monobásico de mag…	1608004-01	1
Caelo	Citrato monobásico de mag…		1
Caelo	Citrato monobásico de mag…	1014E-01829	1
Caelo	Citrato monobásico de mag…	11021401	1
Caelo	Citrato monobásico de mag…	11044103	2
Caelo	Citrato monobásico de mag…	11061403	1
Caelo	Citrato monobásico de mag…	11193104	1
Caelo	Citrato monobásico de mag…	1119I-01829	1
Caelo	Citrato monobásico de mag…	11372901	1
Caelo	Citrato monobásico de mag…	11372902	1
Caelo	Citrato monobásico de mag…	12091303	1
Caelo	Citrato monobásico de mag…	121033-01	1
Caelo	Citrato monobásico de mag…	1214	1
Caelo	Citrato monobásico de mag…	12175801	1
Caelo	Citrato monobásico de mag…	12175802	2
Caelo	Citrato monobásico de mag…	12175807	3
Caelo	Citrato monobásico de mag…	12175810	4
Caelo	Citrato monobásico de mag…	12238002	3
Caelo	Citrato monobásico de mag…	12238004	3
Caelo	Citrato monobásico de mag…	12238012	1
Caelo	Citrato monobásico de mag…	12368002	3
Caelo	Citrato monobásico de mag…	12368003	9
Caelo	Citrato monobásico de mag…	12368004	2
Caelo	Citrato monobásico de mag…	12368005	1
Caelo	Citrato monobásico de mag…	12368011	8
Caelo	Citrato monobásico de mag…	12368014	2
Caelo	Citrato monobásico de mag…	12368017	2
Caelo	Citrato monobásico de mag…	13194601	4
Caelo	Citrato monobásico de mag…	13194603	1
Caelo	Citrato monobásico de mag…	13233901	7
Caelo	Citrato monobásico de mag…	13233904	5
Caelo	Citrato monobásico de mag…	13233905	1
Caelo	Citrato monobásico de mag…	13233906	9
Caelo	Citrato monobásico de mag…	13233907	2
Caelo	Citrato monobásico de mag…	13233910	5
Caelo	Citrato monobásico de mag…	13233911	3
Caelo	Citrato monobásico de mag…	13233913	6
Caelo	Citrato monobásico de mag…	133233907	1
Caelo	Citrato monobásico de mag…	133389111	1
Caelo	Citrato monobásico de mag…	13389103	7
Caelo	Citrato monobásico de mag…	13389106	2
Caelo	Citrato monobásico de mag…	13389107	2
Caelo	Citrato monobásico de mag…	13389108	1
Caelo	Citrato monobásico de mag…	13389111	4
Caelo	Citrato monobásico de mag…	1415013	1
Caelo	Citrato monobásico de mag…	14265503	6
Caelo	Citrato monobásico de mag…	14265504	5
Caelo	Citrato monobásico de mag…	14265505	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato monobásico de mag…	14265511	1
Caelo	Citrato monobásico de mag…	14265513	2
Caelo	Citrato monobásico de mag…	14265514	1
Caelo	Citrato monobásico de mag…	14265516	3
Caelo	Citrato monobásico de mag…	14265517	1
Caelo	Citrato monobásico de mag…	14265520	1
Caelo	Citrato monobásico de mag…	14265521	1
Caelo	Citrato monobásico de mag…	14I12-B02-298854	1
Caelo	Citrato monobásico de mag…	1507010-01	2
Caelo	Citrato monobásico de mag…	15296701	10
Caelo	Citrato monobásico de mag…	15296702	4
Caelo	Citrato monobásico de mag…	15296709	6
Caelo	Citrato monobásico de mag…	15296710	1
Caelo	Citrato monobásico de mag…	15296712	2
Caelo	Citrato monobásico de mag…	15296801	3
Caelo	Citrato monobásico de mag…	15415001	6
Caelo	Citrato monobásico de mag…	15415002	1
Caelo	Citrato monobásico de mag…	15415003	6
Caelo	Citrato monobásico de mag…	15415004	2
Caelo	Citrato monobásico de mag…	15415005	3
Caelo	Citrato monobásico de mag…	15415009	6
Caelo	Citrato monobásico de mag…	15415010	9
Caelo	Citrato monobásico de mag…	15415013	2
Caelo	Citrato monobásico de mag…	15415014	6
Caelo	Citrato monobásico de mag…	15415015	1
Caelo	Citrato monobásico de mag…	160100501	1
Caelo	Citrato monobásico de mag…	1601005-01	1
Caelo	Citrato monobásico de mag…	1604002-01	3
Caelo	Citrato monobásico de mag…	16341707	2
Caelo	Citrato monobásico de mag…	16341708	5
Caelo	Citrato monobásico de mag…	16341709	3
Caelo	Citrato monobásico de mag…	16341710	6
Caelo	Citrato monobásico de mag…	16341711	2
Caelo	Citrato monobásico de mag…	16E02-B03-321485	1
Caelo	Citrato monobásico de mag…	17061401	1
Caelo	Citrato monobásico de mag…	1710007-01	2
Caelo	Citrato monobásico de mag…	17173401	7
Caelo	Citrato monobásico de mag…	17173404	1
Caelo	Citrato monobásico de mag…	17173405	6
Caelo	Citrato monobásico de mag…	17173406	3
Caelo	Citrato monobásico de mag…	17173407	2
Caelo	Citrato monobásico de mag…	17353104	3
Caelo	Citrato monobásico de mag…	17353104P-180831-2	1
Caelo	Citrato monobásico de mag…	17353104P-181001-2	1
Caelo	Citrato monobásico de mag…	17353105	1
Caelo	Citrato monobásico de mag…	17353109	1
Caelo	Citrato monobásico de mag…	1811038-01	2
Caelo	Citrato monobásico de mag…	18216803	4
Caelo	Citrato monobásico de mag…	18216803P-181218-1	1
Caelo	Citrato monobásico de mag…	18216803P-190225-5	1
Caelo	Citrato monobásico de mag…	18216804	3
Caelo	Citrato monobásico de mag…	18216804P-190325-1	1
Caelo	Citrato monobásico de mag…	18216804P-191004-1	1
Caelo	Citrato monobásico de mag…	18216806	6
Caelo	Citrato monobásico de mag…	18274601	1
Caelo	Citrato monobásico de mag…	18274602	1
Caelo	Citrato monobásico de mag…	18274603	2
Caelo	Citrato monobásico de mag…	18274604	3
Caelo	Citrato monobásico de mag…	18274606	3
Caelo	Citrato monobásico de mag…	18274606P-200331-3	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citrato monobásico de mag…	18274609	2
Caelo	Citrato monobásico de mag…	18274610	1
Caelo	Citrato monobásico de mag…	18274612	1
Caelo	Citrato monobásico de mag…	18A08-B04-345115	1
Caelo	Citrato monobásico de mag…	19000684001	2
Caelo	Citrato monobásico de mag…	19000684002	4
Caelo	Citrato monobásico de mag…	19000684003	3
Caelo	Citrato monobásico de mag…	1904011-01	3
Caelo	Citrato monobásico de mag…	19061316	1
Caelo	Citrato monobásico de mag…	20002495002	2
Caelo	Citrato monobásico de mag…	20002495003	4
Caelo	Citrato monobásico de mag…	20002495006	2
Caelo	Citrato monobásico de mag…	20002495010	1
Caelo	Citrato monobásico de mag…	21000135002	1
Caelo	Citrato monobásico de mag…	21000135005	1
Caelo	Citrato monobásico de mag…	21000135006	1
Caelo	Citrato monobásico de mag…	21000135007	2
Caelo	Citrato monobásico de mag…	21000135011	1
Caelo	Citrato monobásico de mag…	21003604004	7
Caelo	Citrato monobásico de mag…	218U-01829	1
Caelo	Citrato monobásico de mag…	2368011	1
Caelo	Citrato monobásico de mag…	26101203	1
Caelo	Citrato monobásico de mag…	27101704	1
Caelo	Citrato monobásico de mag…	27111306	1
Caelo	Citrato monobásico de mag…	315E-01829	1
Caelo	Citrato monobásico de mag…	411052-2-P	1
Caelo	Citrato monobásico de mag…	516Q-01829	1
Caelo	Citrato monobásico de mag…	6081301	1
Caelo	Citrato monobásico de mag…	7011504	1
Caelo	Citrato monobásico de mag…	80446188	1
Caelo	Citrato monobásico de mag…	90396169	1
Caelo	Citrato monobásico de mag…	913M-01829	1
Caeol/Noweda	Citrato monobásico de mag…	17353105	1
Caeolo/Gehe	Citrato monobásico de mag…	17173405	2
Caesar & Loretz GmbH…	Citrato monobásico de mag…	18274602	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	18274601	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	18274609	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	19000684004	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	19000684002	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	20002495003	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	18274609	1
Caesar & Loretz GmbH/Ph	Citrato monobásico de mag…	20002495003	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	20002495002	1
Caesar & Loretz GmbH…	Citrato monobásico de mag…	21000135006	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	17353109	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	18216803	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	18274602	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	18274604	3
Caesar & Loretz GmbH	Citrato monobásico de mag…	18274605	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	18274609	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	18274610	3
Caesar & Loretz GmbH	Citrato monobásico de mag…	19000684003	1
Caesar & Loretz GmbH	Citrato monobásico de mag…	20002495001	2
Caesar & Loretz GmbH	Citrato monobásico de mag…	20002495002	2
Caesar & Loretz GmbH	Citrato monobásico de mag…	20002495003	2
Caesar & Loretz	Citrato monobásico de mag…	16341711	1
Caleo/ Noweda	Citrato monobásico de mag…	18216803	1
Cealo	Citrato monobásico de mag…	12368014	1
Cealo	Citrato monobásico de mag…	13233907	2
Dr. Paul Lohmann	Citrato monobásico de mag…	1077866	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Dr. Paul Lohmann	Citrato monobásico de mag…	1078434	1
Dr. Paul Lohmann	Citrato monobásico de mag…	1079474	1
Eu Rho	Citrato monobásico de mag…	110600401	1
Eu Rho	Citrato monobásico de mag…	1202034-01	1
Eu Rho	Citrato monobásico de mag…	1306034-01	1
EuRho/Phönix	Citrato monobásico de mag…	1202034-02	1
EuRho/Phönix	Citrato monobásico de mag…	1311003-01	1
EuRho	Citrato monobásico de mag…	1311003-02	1
EuRho	Citrato monobásico de mag…	1507010-02	1
EuRho	Citrato monobásico de mag…	1910005-01	1
Euro OTC	Citrato monobásico de mag…		3
Euro OTC	Citrato monobásico de mag…	1080144	1
Euro OTC	Citrato monobásico de mag…	1085730	2
Euro OTC	Citrato monobásico de mag…	1110026-01	2
Euro OTC	Citrato monobásico de mag…	1208006-01	3
Euro OTC	Citrato monobásico de mag…	120800602	1
Euro OTC	Citrato monobásico de mag…	1211033-01	4
Euro OTC	Citrato monobásico de mag…	1211033-02	4
Euro OTC	Citrato monobásico de mag…	1306034-01	2
Euro OTC	Citrato monobásico de mag…	130603402	1
Euro OTC	Citrato monobásico de mag…	1306034-02	2
Euro OTC	Citrato monobásico de mag…	1311003-01	7
Euro OTC	Citrato monobásico de mag…	1311003-02	1
Euro OTC	Citrato monobásico de mag…	140402301	1
Euro OTC	Citrato monobásico de mag…	1404023-01	5
Euro OTC	Citrato monobásico de mag…	140704801	1
Euro OTC	Citrato monobásico de mag…	1407048-01	4
Euro OTC	Citrato monobásico de mag…	1407048-02	3
Euro OTC	Citrato monobásico de mag…	1501026-01	5
Euro OTC	Citrato monobásico de mag…	1507010-01	10
Euro OTC	Citrato monobásico de mag…	1507010-02	2
Euro OTC	Citrato monobásico de mag…	151003301	2
Euro OTC	Citrato monobásico de mag…	1510033-01	2
Euro OTC	Citrato monobásico de mag…	16000456/0	1
Euro OTC	Citrato monobásico de mag…	160100501	1
Euro OTC	Citrato monobásico de mag…	1601005-01	18
Euro OTC	Citrato monobásico de mag…	1604002-001	1
Euro OTC	Citrato monobásico de mag…	1604002-01	34
Euro OTC	Citrato monobásico de mag…	1604002-012x	1
Euro OTC	Citrato monobásico de mag…	1604002-02	8
Euro OTC	Citrato monobásico de mag…	160800401	2
Euro OTC	Citrato monobásico de mag…	1608004-01	22
Euro OTC	Citrato monobásico de mag…	1608004-02	2
Euro OTC	Citrato monobásico de mag…	1701003-01	7
Euro OTC	Citrato monobásico de mag…	170100401	1
Euro OTC	Citrato monobásico de mag…	1701004-01	4
Euro OTC	Citrato monobásico de mag…	17050009-01	1
Euro OTC	Citrato monobásico de mag…	1705009-01	5
Euro OTC	Citrato monobásico de mag…	1705010-01	7
Euro OTC	Citrato monobásico de mag…	1710001-01	1
Euro OTC	Citrato monobásico de mag…	171000701	1
Euro OTC	Citrato monobásico de mag…	1710007-01	10
Euro OTC	Citrato monobásico de mag…	1710007-02	1
Euro OTC	Citrato monobásico de mag…	17353105	1
Euro OTC	Citrato monobásico de mag…	1802026-01	6
Euro OTC	Citrato monobásico de mag…	1808006-01	5
Euro OTC	Citrato monobásico de mag…	1811038-01	11
Euro OTC	Citrato monobásico de mag…	190401101	2
Euro OTC	Citrato monobásico de mag…	1904011-01	15
Euro OTC	Citrato monobásico de mag…	190702001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Citrato monobásico de mag…	1907020-01	7
Euro OTC	Citrato monobásico de mag…	1910005-01	7
Euro OTC	Citrato monobásico de mag…	2003064-01	8
Euro OTC	Citrato monobásico de mag…	2005027-01	14
Euro OTC	Citrato monobásico de mag…	2009007-01	15
Euro OTC	Citrato monobásico de mag…	2101004-01	2
Euro OTC	Citrato monobásico de mag…	2104021-01	1
Euro OTC	Citrato monobásico de mag…	2110009-01	3
Euro OTC	Citrato monobásico de mag…	2114M1829	1
Euro OTC	Citrato monobásico de mag…	220100401	1
Euro OTC	Citrato monobásico de mag…	2201004-01	6
Euro OTC	Citrato monobásico de mag…	2206017-01	6
Euro OTC	Citrato monobásico de mag…	3030559	1
Euro OTC	Citrato monobásico de mag…	3035708	1
Euro OTC	Citrato monobásico de mag…	3068048	1
Fagron	Citrato monobásico de mag…		1
Fagron	Citrato monobásico de mag…	1056239	1
Fagron	Citrato monobásico de mag…	1087537	1
Fagron	Citrato monobásico de mag…	11H05-N07	1
Fagron	Citrato monobásico de mag…	12G10-N01	2
Fagron	Citrato monobásico de mag…	13233901	2
Fagron	Citrato monobásico de mag…	13B22-N03	1
Fagron	Citrato monobásico de mag…	13D30-N07	2
Fagron	Citrato monobásico de mag…	13K11-B02-288161	1
Fagron	Citrato monobásico de mag…	13K11-B02-288161	1
Fagron	Citrato monobásico de mag…	14/12-B02-298854	1
Fagron	Citrato monobásico de mag…	14I12-B02	1
Fagron	Citrato monobásico de mag…	14I12-B02-298854	1
Fagron	Citrato monobásico de mag…	14K-B03-305254	1
Fagron	Citrato monobásico de mag…	15296701	1
Fagron	Citrato monobásico de mag…	16E02-B03-0326874	1
Fagron	Citrato monobásico de mag…	16E02-B03-326874	1
Fagron	Citrato monobásico de mag…	17G24-B03-338029	2
Fagron	Citrato monobásico de mag…	17G24-B03-341019	1
Fagron	Citrato monobásico de mag…	18/20-B06	1
Fagron	Citrato monobásico de mag…	18A08-B04-345115	1
Fagron	Citrato monobásico de mag…	18A08-B04-345155	1
Fagron	Citrato monobásico de mag…	18A08-B04-349372	1
Fagron	Citrato monobásico de mag…	18I20-B06-355658	1
Fagron	Citrato monobásico de mag…	20A17-B08-196635	2
Fagron	Citrato monobásico de mag…	20A17-B08-200819	1
Fagron	Citrato monobásico de mag…	20I25-B03-201926	1
Fagron	Citrato monobásico de mag…	3047166	2
Fagron	Citrato monobásico de mag…	B07-2136601	1
Fiebig	Citrato monobásico de mag…	1802026-01	1
Gatt-Koller	Citrato monobásico de mag…		1
Gatt-Koller	Citrato monobásico de mag…	1800208	1
Gatt-Koller	Citrato monobásico de mag…	1802721	1
Gatt-Koller	Citrato monobásico de mag…	1803714	2
Gehe Kassel	Citrato monobásico de mag…	14/12-B02-298854	1
GEHE	Citrato monobásico de mag…	1802026-01	1
Heidelberger Chlorel…	Citrato monobásico de mag…	10032	1
Heidelberger Chlorella	Citrato monobásico de mag…	90196	1
Ichthyol/Phönix	Citrato monobásico de mag…	14/12-B02-298854	1
INTERN-DROGEN	Citrato monobásico de mag…	210001350007	1
INTERN-DROGEN	Citrato monobásico de mag…	21000135006	1
Kehr	Citrato monobásico de mag…	17173406	1
kögl	Citrato monobásico de mag…	1900910	1
L30	Citrato monobásico de mag…	1608004-01	1
lohmann	Citrato monobásico de mag…	3054132	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Nachprüfung vom 31.1…	Citrato monobásico de mag…	16341710	1
Nowed18.08.2015	Citrato monobásico de mag…	14265521	1
Noweda	Citrato monobásico de mag…	10163306	1
Noweda	Citrato monobásico de mag…	16341710	1
Noweda	Citrato monobásico de mag…	18274603	1
Noweda	Citrato monobásico de mag…	2005027-01	1
Noweda	Citrato monobásico de mag…	22002876002	1
Noweda	Citrato monobásico de mag…	2206017-01	1
Phoenix 15.10.14	Citrato monobásico de mag…	1311003-01	1
Phönix	Citrato monobásico de mag…	1211033-01	2
phönix	Citrato monobásico de mag…	15296702	1
phönix	Citrato monobásico de mag…	15296710	1
Phönix	Citrato monobásico de mag…	15415005	1
phönix	Citrato monobásico de mag…	15415010	1
phönix	Citrato monobásico de mag…	15415015	2
phönix	Citrato monobásico de mag…	1601005-01	2
phönix	Citrato monobásico de mag…	1604002-01	1
phönix	Citrato monobásico de mag…	1608004-01	1
phönix	Citrato monobásico de mag…	16341709	2
Sanacaorp	Citrato monobásico de mag…	13389108	1
Sanacorp	Citrato monobásico de mag…	16341710	1
Sanacorp	Citrato monobásico de mag…	20002495003	1
Sanacorp	Citrato monobásico de mag…	20A17-B08-196635	1
Sanacorp	Citrato monobásico de mag…	22001882001	1
Sanacorp	Citrato monobásico de mag…	2304016-01	1
Sanacorp	Citrato monobásico de mag…	3108363	1
VDL;27.02.15	Citrato monobásico de mag…	13389111	1

- 235 256 spectra from 1515 *Apo-Ident* customers from a total of 49 007 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrato monobásico de magnésio, hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrato monobásico de magnésio, hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	1490	0	200 594
Type C	0	810	1	235 256

The substance/substance group *Citrato monobásico de magnésio, hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5973 %)
Type C	100.0000 % (> 99.9007 %)	99.8767 % (> 99.5068 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21445	22233	5,57	88,08
21873	21873	0,00	86,27
22233	22233	0,00	87,51
22296	22296	0,00	87,45
22992	22992	0,00	85,89
23240	22992	4,21	85,88
25545	25545	0,00	94,75
26251	26251	0,00	78,03
26400	26400	0,00	114,13
26423	26423	0,00	90,20
27302	21873	40,54	99,56

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrulina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21095-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrulina; Citrullinum

Special notes

When selecting the *Citrulina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrulina	9	11	22

Second-stage model

For differentiation of the substance/substance group *Citrulina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrulina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	93,45	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrulina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrulina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Citrulina	1310015-01	21095	40	20131120
Euro OTC	Citrulina	1403021-01	21565	59	1411031
Euro OTC	Citrulina	1604038	22560	40	20160523*
Euro OTC	Citrulina	1703036	23175	40	20170418*
Euro OTC	Citrulina	1811028	24348	40	20181127*
Euro OTC	Citrulina	2003033	25415	40	20200914*
Euro OTC	Citrulina	2011009	25462	40	20201126*
Fagron	Citrulina	16D11-B02-326797	23567	40	20160421
Fagron	Citrulina	18K15-B01-356962	24643	40	20190123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 379 spectra of 9 reference samples from the substance/substance group *Citrulina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 583 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 510 spectra of 14 reference samples from the substance/substance group *Citrulina*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Citrulina	1609013	22866	40
Euro OTC	Citrulina	1707003	23538	40
Euro OTC	Citrulina	1710039	23913	40
Euro OTC	Citrulina	1805028	24117	40
Euro OTC	Citrulina	1904013	24627	40
Euro OTC	Citrulina	2001002	25070	40
Euro OTC	Citrulina	2109012	25827	50
Euro OTC	Citrulina	2301010	26517	40
Euro OTC	Citrulina	2401009	27163	40
Fagron	Citrulina	19E03-B01-362002	24819	40
Fagron	Citrulina	22G22-B05-222418	26375	40
Euro OTC	Citrulina	2301010	26517SI	20
Euro OTC	Citrulina	2401009	27163SI	20
Fagron	Citrulina	22G22-B05-222418	26375SI	20

- 201 574 spectra from a total of 4034 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 9 *Apo-Ident* customers from 23 batches from the substance/substance group *Citrulina*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Citrulina	17C14-B01-339452	2
Dr. Schär	Citrulina	R1216-022A	1
Dr.Schär GmbH (Direkt)	Citrulina	20190700	1
Dr.Schär GmbH (Direkt)	Citrulina	20200027	1
Euro OTC	Citrulina	16040038-01	1
Euro OTC	Citrulina	1811028-01	1
Euro OTC	Citrulina	1904013-01	2
Euro OTC	Citrulina	2001002-01	3
Euro OTC	Citrulina	20011002-01	1
Euro OTC	Citrulina	2003033-01	3
Euro OTC	Citrulina	2011009-01	2
Euro OTC	Citrulina	2109012-01	1
Euro OTC	Citrulina	CIT-PL-19102	1
Fagron	Citrulina	18B12-B02	1
Fagron	Citrulina	18K15-B01	1
Fagron	Citrulina	19M17F01366482	1
Fagron	Citrulina	20A28-F02-368558	1
Fagron	Citrulina	21C08-F05-377311	2
Gall-Pharma GmbH/Noweda	Citrulina		1
Gall-Pharma GmbH	Citrulina		1
Hecht-Pharma/ Noweda	Citrulina		1
Nutricia	Citrulina	100803609	1
Nutricia	Citrulina	100915050	2

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrulina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrulina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	379	0	152 583
Type B	0	510	0	201 574
Type C	0	31	1	236 035

The substance/substance group *Citrulina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4169 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8235 %)
Type C	100.0000 % (> 99.9007 %)	96.8750 % (> 87.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21095	21565	9,88	131,20
21565	21565	0,00	127,86
22560	22560	0,00	138,37
23175	23175	0,00	142,33
23567	22560	4,78	140,79
24348	24348	0,00	126,86
24643	25462	5,50	137,08
25415	25415	0,00	144,00
25462	25462	0,00	136,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clioquinol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20095-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clioquinol; Clioquinolum

Special notes

When selecting the *Clioquinol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clioquinol	7	13	344

Second-stage model

For differentiation of the substance/substance group *Clioquinol* the following second-stage model is used:

- Submodelo 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clioquinol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	114,58	–
⋮	⋮	⋮
Mesalazina	>50	25,56
Nitrato de miconazol	>50	41,94
Teofilina etilenodiamina hidratada	>50	60,48
Ácido nicotínico	>50	76,82

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clioquinol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clioquinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clioquinol	11304120	20895	40	20111208
Caelo	Clioquinol	163072	23047	40	20161202*
Euro OTC	Clioquinol	1309009-02	21246	40	AR-15-FG-009542-01
Euro OTC	Clioquinol	1509038	21944	60	20151009*
Euro OTC	Clioquinol	2309015	27002	40	20231120*
Fagron	Clioquinol	13I26-N15	21236	40	20131028
Fagron	Clioquinol	14I11-B03-300049	21913	60	20140926
Fagron	Clioquinol	14I11-B03-300049	21972	60	20140926

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 380 spectra of 8 reference samples from the substance/substance group *Clioquinol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 582 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 570 spectra of 16 reference samples from the substance/substance group *Clioquinol*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clioquinol	13114413	21308	40
Caelo	Clioquinol	16307206	22960	40
Caelo	Clioquinol	172046	23633	40
Caelo	Clioquinol	182782	24374	40
Caelo	Clioquinol	21000089	25923	40
Caelo	Clioquinol	22000908001	26413	40
Caelo	Clioquinol	23000424	26850	40
Euro OTC	Clioquinol	1612020	22985	40
Euro OTC	Clioquinol	1903010	24624	40
Euro OTC	Clioquinol	1910030	24968	40
Euro OTC	Clioquinol	2011013	25566	40
Euro OTC	Clioquinol	2208002	26268	40
Fagron	Clioquinol	21J01-B08-218979	26159	40
Caelo	Clioquinol	21000089	25923SI	10
Euro OTC	Clioquinol	2208002	26268SI	20
Fagron	Clioquinol	21J01-B08-218979	26159SI	20

- 201 514 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1991 spectra from 825 *Apo-Ident* customers from 356 batches from the substance/substance group *Clioquinol*.
- Among them are spectra of independent samples from 344 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clioquinol	22000908001	1
	Clioquinol	22000908003	2
	Clioquinol	22000908007	2
	Clioquinol	22000908008	3
	Clioquinol	22000908011	1
	Clioquinol	22000908012	10
	Clioquinol	220009098008	1
	Clioquinol	22001088008	1
	Clioquinol	2208002-01	6
	Clioquinol	2208002-02	2
	Clioquinol	22G25-B03-227776	2
	Clioquinol	22G25-B03-2278803	1
	Clioquinol	23000424001	20
	Clioquinol	23000424003	1
	Clioquinol	23000424004	1
	Clioquinol	23000424007	4
	Clioquinol	23003409006	3
	Clioquinol	2300424001	1
	Clioquinol	2300424003	1
	Clioquinol	8069D22	2
	Clioquinol	B03-2277706	1
aelo/Noweda	Clioquinol	21000089001	1
AHD	Clioquinol	1612020-01	1
AHD	Clioquinol	18011502	1
AHD	Clioquinol	2011013-01	1
AHD	Clioquinol	2208002	1
Alliance Healthcare	Clioquinol	19120-B01-196485	1
Alliance Healthcare	Clioquinol	22000908001	1
Alliance	Clioquinol	182782002	1
Alliance	Clioquinol	2011013-01	1
Alliance	Clioquinol	22000908001	1
Alliance	Clioquinol	2205002-01	1
Alliance	Clioquinol	23000424001	1
Anzag	Clioquinol	12L04-N08	1
anzag	Clioquinol	13114418	1
Anzag	Clioquinol	18011517	3
Anzag	Clioquinol	18278210	1
Anzag	Clioquinol	22001088008	1
Anzag	Clioquinol	23000424001	3
Anzag	Clioquinol	23000424003	1
Apo-ident	Clioquinol	1509038-02	1
apo-ident	Clioquinol	1612020-02	1
apomix	Clioquinol	1509038-02	1
Axyntis Group	Clioquinol	1301014-02	1
Axyntis Group	Clioquinol	1301014-03	1
Axyntis Group	Clioquinol	1612020-02	1
Axyntis Group	Clioquinol	F001461	1
Bombastus	Clioquinol	14359118	1
Bombastus	Clioquinol	1509038-03	1
Bombastus	Clioquinol	1903010-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cael Sanacorp 05.02.2016	Clioquinol	14359103	1
Caelo	Clioquinol	103415	2
Caelo	Clioquinol	10341510	1
Caelo	Clioquinol	10341601	2
Caelo	Clioquinol	10341605	4
Caelo	Clioquinol	10341608	1
Caelo	Clioquinol	11(18011523)	1
Caelo	Clioquinol	1130312	1
Caelo	Clioquinol	11304102	7
Caelo	Clioquinol	11304103	2
Caelo	Clioquinol	11304105	3
Caelo	Clioquinol	11304107	5
Caelo	Clioquinol	11304109	1
Caelo	Clioquinol	11304111	2
Caelo	Clioquinol	11304112	6
Caelo	Clioquinol	11304113	4
Caelo	Clioquinol	11304116	3
Caelo	Clioquinol	11304117	10
Caelo	Clioquinol	11304119	3
Caelo	Clioquinol	11304120	12
Caelo	Clioquinol	11304124	13
Caelo	Clioquinol	1201034-01	1
Caelo	Clioquinol	1201034-02	2
Caelo	Clioquinol	1214I02562	1
Caelo	Clioquinol	12F20-N05	1
Caelo	Clioquinol	12L04-N08	2
Caelo	Clioquinol	130114-02	1
Caelo	Clioquinol	1309009-02	1
Caelo	Clioquinol	13114404	2
Caelo	Clioquinol	13114406	1
Caelo	Clioquinol	13114408	3
Caelo	Clioquinol	13114410	2
Caelo	Clioquinol	13114413	11
Caelo	Clioquinol	13114415	3
Caelo	Clioquinol	13114417	7
Caelo	Clioquinol	13114418	5
Caelo	Clioquinol	13114421	1
Caelo	Clioquinol	13114422	7
Caelo	Clioquinol	13114423	10
Caelo	Clioquinol	13114424	10
Caelo	Clioquinol	13114427	2
Caelo	Clioquinol	13A29-N07	1
Caelo	Clioquinol	14/11-B03-309181	1
Caelo	Clioquinol	14/11-BG03-309181	1
Caelo	Clioquinol	14/-B03-309181	1
Caelo	Clioquinol	1405080031	1
Caelo	Clioquinol	1405080036	1
Caelo	Clioquinol	1409031-01	1
Caelo	Clioquinol	14353120	1
Caelo	Clioquinol	14359102	12
Caelo	Clioquinol	14359103	11
Caelo	Clioquinol	14359111	14
Caelo	Clioquinol	14359112	14
Caelo	Clioquinol	14359113	2
Caelo	Clioquinol	14359116	1
Caelo	Clioquinol	14359117	4
Caelo	Clioquinol	14359118	10
Caelo	Clioquinol	14359119	4
Caelo	Clioquinol	14359120	8
Caelo	Clioquinol	1435918	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clioquinol	144359111	1
Caelo	Clioquinol	14C21-B06-293104	1
Caelo	Clioquinol	1509038-01	1
Caelo	Clioquinol	1509038-02	3
Caelo	Clioquinol	150903803	1
Caelo	Clioquinol	1509038-03	4
Caelo	Clioquinol	1509038-OTC-Pharma	1
Caelo	Clioquinol	15L30-B05-314974	1
Caelo	Clioquinol	15L30-B05-321899	2
Caelo	Clioquinol	16021505	1
Caelo	Clioquinol	1605100084	1
Caelo	Clioquinol	160916CL	1
Caelo	Clioquinol	1612020-01	8
Caelo	Clioquinol	1612020-02	1
Caelo	Clioquinol	1612020-03	1
Caelo	Clioquinol	16122020-01	1
Caelo	Clioquinol	163072	1
Caelo	Clioquinol	16307203	3
Caelo	Clioquinol	16307204	1
Caelo	Clioquinol	16307205	14
Caelo	Clioquinol	16307206	23
Caelo	Clioquinol	16307207	23
Caelo	Clioquinol	163072073	1
Caelo	Clioquinol	16307208	17
Caelo	Clioquinol	16307209	1
Caelo	Clioquinol	16307210	6
Caelo	Clioquinol	16307211	9
Caelo	Clioquinol	16307213	1
Caelo	Clioquinol	16307214	18
Caelo	Clioquinol	16307215	15
Caelo	Clioquinol	16307216	18
Caelo	Clioquinol	16I18-B04-332852	1
Caelo	Clioquinol	16J18-B04-328520	1
Caelo	Clioquinol	16l18-B04-329141	1
Caelo	Clioquinol	170926CL/16307208	1
Caelo	Clioquinol	172041603	1
Caelo	Clioquinol	17204601	4
Caelo	Clioquinol	17204603	22
Caelo	Clioquinol	172046303	1
Caelo	Clioquinol	18011501	2
Caelo	Clioquinol	18011502	48
Caelo	Clioquinol	18011511	2
Caelo	Clioquinol	180115117	1
Caelo	Clioquinol	18011516	39
Caelo	Clioquinol	18011516P-190705-1	1
Caelo	Clioquinol	18011517	2
Caelo	Clioquinol	18011523	30
Caelo	Clioquinol	18011527	1
Caelo	Clioquinol	180127C/16307215	1
Caelo	Clioquinol	1801523	1
Caelo	Clioquinol	18121714	1
Caelo	Clioquinol	1827782008	1
Caelo	Clioquinol	18278002	1
Caelo	Clioquinol	182782002	43
Caelo	Clioquinol	182782003	1
Caelo	Clioquinol	182782007	1
Caelo	Clioquinol	182782008	15
Caelo	Clioquinol	182782009	15
Caelo	Clioquinol	18278202	4
Caelo	Clioquinol	18278205	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clioquinol	18278206	22
Caelo	Clioquinol	18278210	9
Caelo	Clioquinol	18278214	29
Caelo	Clioquinol	18278215	24
Caelo	Clioquinol	182792008	1
Caelo	Clioquinol	18E08-B06-355575	2
Caelo	Clioquinol	19I2O-B01-196485	1
Caelo	Clioquinol	20001561001	2
Caelo	Clioquinol	20001561003	6
Caelo	Clioquinol	20001561006	5
Caelo	Clioquinol	2001561001	2
Caelo	Clioquinol	2011013-01	1
Caelo	Clioquinol	21000089001	50
Caelo	Clioquinol	21000089004	5
Caelo	Clioquinol	21000089006	28
Caelo	Clioquinol	2100008901	2
Caelo	Clioquinol	21000089011	21
Caelo	Clioquinol	21000089015	3
Caelo	Clioquinol	210000899004	1
Caelo	Clioquinol	21000098006	1
Caelo	Clioquinol	2100089001	1
Caelo	Clioquinol	22000308003	1
Caelo	Clioquinol	220009080001	1
Caelo	Clioquinol	220009080003	1
Caelo	Clioquinol	22000908001	19
Caelo	Clioquinol	22000908003	4
Caelo	Clioquinol	22000908008	6
Caelo	Clioquinol	22000908011	1
Caelo	Clioquinol	22000908012	1
Caelo	Clioquinol	22001088003	10
Caelo	Clioquinol	22001088004	1
Caelo	Clioquinol	23000424001	1
Caelo	Clioquinol	2773	1
Caelo	Clioquinol	3041409	1
Caelo	Clioquinol	3513I-02562	1
Caelo	Clioquinol	3713A2562	1
Caelo	Clioquinol	4111707	1
Caelo	Clioquinol	4214Q-02562	1
Caelo	Clioquinol	4613E2562	1
Caelo	Clioquinol	5031302	1
Caelo	Clioquinol	5089	1
Caelo	Clioquinol	5213A2562	1
Caelo	Clioquinol	8714	1
Caelo	Clioquinol	B01-1964805	1
Caesar & Lorenz GmbH	Clioquinol	14359112	1
Caesar & Loretz GmbH…	Clioquinol	21000089004	1
Caesar & Loretz GmbH…	Clioquinol	21000089001	1
Caesar & Loretz GmbH…	Clioquinol	21000089006	1
Caesar & Loretz GmbH…	Clioquinol	22001088003	1
Caesar & Loretz GmbH…	Clioquinol	18278214	2
Caesar & Loretz GmbH…	Clioquinol	18278215	1
Caesar & Loretz GmbH…	Clioquinol	21000089001	3
Caesar & Loretz GmbH…	Clioquinol	21000089001	1
Caesar & Loretz GmbH/AEP	Clioquinol	21000089012	1
Caesar & Loretz GmbH/AHD	Clioquinol	18011523	1
Caesar & Loretz GmbH/AHD	Clioquinol	22000908008	1
Caesar & Loretz GmbH/AHD	Clioquinol	22001088003	1
Caesar & Loretz GmbH/Alli	Clioquinol	18278215	1
Caesar & Loretz GmbH…	Clioquinol	21000089001	1
Caesar & Loretz GmbH…	Clioquinol	18011502	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH/Gehe	Clioquinol	182782002	1
Caesar & Loretz GmbH/Gehe	Clioquinol	21000089006	1
Caesar & Loretz GmbH/Gehe	Clioquinol	22001088004	2
Caesar & Loretz GmbH/Gehe	Clioquinol	23000424001	2
Caesar & Loretz GmbH...	Clioquinol	22000908003	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089004	1
Caesar & Loretz GmbH...	Clioquinol	22001088008	1
Caesar & Loretz GmbH/K	Clioquinol	182782009	1
Caesar & Loretz GmbH/Kehr	Clioquinol	182782008	1
Caesar & Loretz GmbH...	Clioquinol	18278202	1
Caesar & Loretz GmbH/Ph	Clioquinol	18278214	1
Caesar & Loretz GmbH...	Clioquinol	20001561006	1
Caesar & Loretz GmbH...	Clioquinol	22000908001	1
Caesar & Loretz GmbH...	Clioquinol	182782008	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089015	1
Caesar & Loretz GmbH...	Clioquinol	22000908008	2
Caesar & Loretz GmbH...	Clioquinol	182782008	1
Caesar & Loretz GmbH...	Clioquinol	182782009	1
Caesar & Loretz GmbH...	Clioquinol	18278214	1
Caesar & Loretz GmbH...	Clioquinol	20001561006	1
Caesar & Loretz GmbH...	Clioquinol	21000089011	1
Caesar & Loretz GmbH...	Clioquinol	22001088004	1
Caesar & Loretz GmbH	Clioquinol	1612020-02	1
Caesar & Loretz GmbH	Clioquinol	16307207	1
Caesar & Loretz GmbH	Clioquinol	16307216	1
Caesar & Loretz GmbH	Clioquinol	18011516	5
Caesar & Loretz GmbH	Clioquinol	18011517	3
Caesar & Loretz GmbH	Clioquinol	18011523	3
Caesar & Loretz GmbH	Clioquinol	18273214	1
Caesar & Loretz GmbH	Clioquinol	182778215	1
Caesar & Loretz GmbH	Clioquinol	182782002	10
Caesar & Loretz GmbH	Clioquinol	182782003	1
Caesar & Loretz GmbH	Clioquinol	182782006	1
Caesar & Loretz GmbH	Clioquinol	182782008	5
Caesar & Loretz GmbH	Clioquinol	182782009	3
Caesar & Loretz GmbH	Clioquinol	18278202	1
Caesar & Loretz GmbH	Clioquinol	18278206	2
Caesar & Loretz GmbH	Clioquinol	18278210	2
Caesar & Loretz GmbH	Clioquinol	18278214	11
Caesar & Loretz GmbH	Clioquinol	18278215	5
Caesar & Loretz GmbH	Clioquinol	20001561003	1
Caesar & Loretz GmbH	Clioquinol	20001561006	2
Caesar & Loretz GmbH	Clioquinol	21000089001	11
Caesar & Loretz GmbH	Clioquinol	21000089004	2
Caesar & Loretz GmbH	Clioquinol	21000089006	12
Caesar & Loretz GmbH	Clioquinol	21000089011	2
Caesar & Loretz GmbH	Clioquinol	21000089012	2
Caesar & Loretz GmbH	Clioquinol	21000089015	2
Caesar & Loretz GmbH	Clioquinol	22000908001	8
Caesar & Loretz GmbH	Clioquinol	22000908003	2
Caesar & Loretz GmbH	Clioquinol	22001088003	5
Caesar & Loretz GmbH	Clioquinol	22001088004	2
Caesar & Loretz Hilden	Clioquinol	18011516	1
Caesar & Loretz Hilden	Clioquinol	18011523	1
Caesar & Loretz/Noweda	Clioquinol	182782008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz	Clioquinol	18011502	1
Caesar&Lorenz	Clioquinol	2100089001	1
caesar&loretz,Phönix	Clioquinol	14359111	1
Caolo- Noweda	Clioquinol	14359118	1
Cealo/ Anzag	Clioquinol	16307215	1
Cealo/Sanacorp	Clioquinol	1309009-01	1
Cealo/Sanacorp	Clioquinol	18278206	1
Ebert & Jacobi	Clioquinol	14359103	1
EuRho / Gehe	Clioquinol	1910030-01	2
EuRho/Gehe	Clioquinol	1910030-02	2
EuRho/Phönix	Clioquinol	1903010-01	1
Eurho/Phönix	Clioquinol	1910030-01	1
Eurho/Phönix	Clioquinol	201101301	1
EuRho	Clioquinol	1201034-02	1
EuRho	Clioquinol	1309009-02	1
EuRho	Clioquinol	161202001	1
EuRho	Clioquinol	1612020-01	1
EuRho	Clioquinol	1612020-02	1
EuRho	Clioquinol	1910030-02	1
Eurho	Clioquinol	2011013-01	1
EuRho	Clioquinol	201101301	1
EuRho	Clioquinol	2011013-01	3
EURO / Sanacorp	Clioquinol	150903802	1
Euro OTC	Clioquinol		1
Euro OTC	Clioquinol	1102022-01	2
Euro OTC	Clioquinol	1102022-02	3
Euro OTC	Clioquinol	1201034-01	5
Euro OTC	Clioquinol	120103402	1
Euro OTC	Clioquinol	1201034-02	8
Euro OTC	Clioquinol	1213A-02562	1
Euro OTC	Clioquinol	13010104-03	1
Euro OTC	Clioquinol	1301014	1
Euro OTC	Clioquinol	1301014-01	2
Euro OTC	Clioquinol	1301014-02	6
Euro OTC	Clioquinol	1301041-01	1
Euro OTC	Clioquinol	1303009-02	1
Euro OTC	Clioquinol	1305070109	1
Euro OTC	Clioquinol	1309009-01	7
Euro OTC	Clioquinol	130900902	1
Euro OTC	Clioquinol	1309009-02	14
Euro OTC	Clioquinol	1405080031	1
Euro OTC	Clioquinol	14090131-02	1
Euro OTC	Clioquinol	140903101	1
Euro OTC	Clioquinol	1409031-01	5
Euro OTC	Clioquinol	1409031-02	11
Euro OTC	Clioquinol	14359118	1
Euro OTC	Clioquinol	14359120	1
Euro OTC	Clioquinol	150903-01	1
Euro OTC	Clioquinol	1509038	2
Euro OTC	Clioquinol	1509038-0	1
Euro OTC	Clioquinol	1509038-01	13
Euro OTC	Clioquinol	150903802	2
Euro OTC	Clioquinol	1509038-02	40
Euro OTC	Clioquinol	1509038-03	30
Euro OTC	Clioquinol	150903804	1
Euro OTC	Clioquinol	1509038-04	5
Euro OTC	Clioquinol	1509038-31	1
Euro OTC	Clioquinol	1605100084	1
Euro OTC	Clioquinol	1612020	3
Euro OTC	Clioquinol	1612020_01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clioquinol	161202001	3
Euro OTC	Clioquinol	1612020-01	44
Euro OTC	Clioquinol	1612020-02	20
Euro OTC	Clioquinol	161202003	1
Euro OTC	Clioquinol	1612020-03	26
Euro OTC	Clioquinol	1612022001	1
Euro OTC	Clioquinol	16307208	1
Euro OTC	Clioquinol	16307216	1
Euro OTC	Clioquinol	16J18-B04	1
Euro OTC	Clioquinol	1903010	1
Euro OTC	Clioquinol	1903010-01	10
Euro OTC	Clioquinol	19100030-02	1
Euro OTC	Clioquinol	1910020-01	1
Euro OTC	Clioquinol	1910030	2
Euro OTC	Clioquinol	19100300-01	1
Euro OTC	Clioquinol	191003001	2
Euro OTC	Clioquinol	1910030-01	18
Euro OTC	Clioquinol	191003002	3
Euro OTC	Clioquinol	1910030-02	24
Euro OTC	Clioquinol	2011013-01	30
Euro OTC	Clioquinol	211013-01	1
Euro OTC	Clioquinol	2195137	1
Euro OTC	Clioquinol	22022021-1	1
Euro OTC	Clioquinol	2208002-01	6
Euro OTC	Clioquinol	2507212562	1
Euro OTC	Clioquinol	3719U-02562	1
Euro OTC	Clioquinol	5219E32562	1
Euro OTC	Clioquinol	PC86	1
Euro OTC	Clioquinol	RetestCharge24619/3	1
Euro/Phoenix	Clioquinol	1612020-02	3
Euro/Phönix	Clioquinol	1509038-02	1
Euro	Clioquinol	1509038-01	2
EuRoh	Clioquinol	2011013-01	2
europharm	Clioquinol	1509038	1
Fagron	Clioquinol		1
Fagron	Clioquinol	1005090024	1
Fagron	Clioquinol	11304112	1
Fagron	Clioquinol	11304120	1
Fagron	Clioquinol	11G20/N09	1
Fagron	Clioquinol	11G20-N09	1
Fagron	Clioquinol	11K21-N18	4
Fagron	Clioquinol	1205110014	1
Fagron	Clioquinol	12F20-N05	3
Fagron	Clioquinol	12L04-N08	7
Fagron	Clioquinol	13/26-N15	2
Fagron	Clioquinol	1305120028	1
Fagron	Clioquinol	1309009-01	1
Fagron	Clioquinol	13114417	1
Fagron	Clioquinol	13114423	2
Fagron	Clioquinol	13114424	1
Fagron	Clioquinol	1326-N15	3
Fagron	Clioquinol	13A29-N07	7
Fagron	Clioquinol	13A29-N07-3398310111	1
Fagron	Clioquinol	13D15-N01	8
Fagron	Clioquinol	13DS15-NO1	1
Fagron	Clioquinol	13F12-N20	2
Fagron	Clioquinol	13F12-N200463480	1
Fagron	Clioquinol	13I26N15	1
Fagron	Clioquinol	13I26-N15	5
Fagron	Clioquinol	14/11-803-309181	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clioquinol	14/11-B03-300049	3
Fagron	Clioquinol	14/11-B03-309181	4
Fagron	Clioquinol	14/11-Bo3	1
Fagron	Clioquinol	14052014C	1
Fagron	Clioquinol	1411-813	1
Fagron	Clioquinol	1411B03300049	1
Fagron	Clioquinol	1411-B03-300049	4
Fagron	Clioquinol	1411-B03-309181	1
Fagron	Clioquinol	14359118	1
Fagron	Clioquinol	14C21806293104	1
Fagron	Clioquinol	14C21-B06	2
Fagron	Clioquinol	14c21B06293104	1
Fagron	Clioquinol	14C21B06293104	1
Fagron	Clioquinol	14C21-B06-293104	6
Fagron	Clioquinol	14C21-B06-293132	2
Fagron	Clioquinol	14-C21-B06-293132	1
Fagron	Clioquinol	14C21-B06-297159	3
Fagron	Clioquinol	14C21-B08	1
Fagron	Clioquinol	14I11-B03	2
Fagron	Clioquinol	14I11-B03-3000049	1
Fagron	Clioquinol	14I11B03300049	1
Fagron	Clioquinol	14I11-B03-300049	6
Fagron	Clioquinol	14I11-B03-309048	2
Fagron	Clioquinol	14I11-B03-309181	3
Fagron	Clioquinol	14L11-B03	1
Fagron	Clioquinol	14l11-B03-300049	1
Fagron	Clioquinol	1505120044	1
Fagron	Clioquinol	15L30-321899	1
Fagron	Clioquinol	15L30-B05	2
Fagron	Clioquinol	15L30-B05-314974	8
Fagron	Clioquinol	15L30-B05-319616	2
Fagron	Clioquinol	15L30-B05-321899	7
Fagron	Clioquinol	15L30-B05-321899	1
Fagron	Clioquinol	16/18-b04-328511	1
Fagron	Clioquinol	16/18-B04-328511	1
Fagron	Clioquinol	16/18-B04-332852	2
Fagron	Clioquinol	1605100008	2
Fagron	Clioquinol	1612020-03	1
Fagron	Clioquinol	1618B04-329141	1
Fagron	Clioquinol	16J18B04	1
Fagron	Clioquinol	16J18-B04	2
Fagron	Clioquinol	16J18-B04-328511	8
Fagron	Clioquinol	16J18-B04-328520	2
Fagron	Clioquinol	16J18-B04-32914	1
Fagron	Clioquinol	16j18-b04-329141	1
Fagron	Clioquinol	16j18-B04-329141	1
Fagron	Clioquinol	16J18B04329141	1
Fagron	Clioquinol	16J18-B04-329141	4
Fagron	Clioquinol	16J18-B04-329704	1
Fagron	Clioquinol	16J18-B04-332852	6
Fagron	Clioquinol	16J18-B04-332861	1
Fagron	Clioquinol	17204603	1
Fagron	Clioquinol	18805B07345488	1
Fagron	Clioquinol	18805-B07-3475B6	1
Fagron	Clioquinol	188B05-B07345483	1
Fagron	Clioquinol	18B05-B07	2
Fagron	Clioquinol	18B05-B07-345483	3
Fagron	Clioquinol	18B05-B07-345488	2
Fagron	Clioquinol	18B05-B07-347586	3
Fagron	Clioquinol	18E08-B06	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clioquinol	18E08-B06-350976	2
Fagron	Clioquinol	18E08-B06-352127	4
Fagron	Clioquinol	18E08-B06-355552	2
Fagron	Clioquinol	18E08-B06355575	1
Fagron	Clioquinol	18E08-B06-355575	2
Fagron	Clioquinol	19/20-B01-196485	1
Fagron	Clioquinol	19/20-B01-197294	1
Fagron	Clioquinol	19F17B07-191238	1
Fagron	Clioquinol	19F17-B07-191238	2
Fagron	Clioquinol	19F17-B07-191238/08122I18	1
Fagron	Clioquinol	19F17-B07-191239	3
Fagron	Clioquinol	19I20-B01-196485	4
Fagron	Clioquinol	19I20-B01-1972904	1
Fagron	Clioquinol	19I20-B01-197294	3
Fagron	Clioquinol	19I20-B01-197295	3
Fagron	Clioquinol	19I20-Bo1-196485	1
Fagron	Clioquinol	19l20-B01-196485	1
Fagron	Clioquinol	2011013-01	1
Fagron	Clioquinol	2014Q2562	1
Fagron	Clioquinol	21D01-B08-217230	1
Fagron	Clioquinol	21G22-B05-213512	1
Fagron	Clioquinol	21J01-B08-218979	1
Fagron	Clioquinol	21J01-B08-219069	1
Fagron	Clioquinol	22C15-B07-220931	4
Fagron	Clioquinol	22C15-B07-223056	2
Fagron	Clioquinol	22G25-B03-222915	2
Fagron	Clioquinol	22G25B03227776	1
Fagron	Clioquinol	22G25-B03-227776	1
Fagron	Clioquinol	2514U2562	1
Fagron	Clioquinol	28031401	1
Fagron	Clioquinol	3916U-02562	1
Fagron	Clioquinol	7D20-N03	1
Fagron	Clioquinol	812218	1
Fagron	Clioquinol	8122I18	1
Fagron	Clioquinol	B01-1964805	1
Fagron	Clioquinol	B01-1972904	1
Fargon	Clioquinol	16J18-B04-329704	1
Fiebig	Clioquinol	14/11-B03-300048	1
Fiebig	Clioquinol	1409031-02	2
Fiebig	Clioquinol	19I20-B01-196485	1
Gatt-Koller	Clioquinol	1802295	2
GEHE 04.08.2014	Clioquinol	13114418	1
Gehe amax	Clioquinol	13114418	1
Gehe/EuRho	Clioquinol	1910030-01	1
Gehe	Clioquinol	1409031-02	1
GEHE	Clioquinol	1509038-02	1
Gehe	Clioquinol	1509038-03	1
GEHE	Clioquinol	1509038-03	1
Gehe	Clioquinol	1612020-01	1
Gehe	Clioquinol	16307216	1
Gehe	Clioquinol	18011502	1
GEHE	Clioquinol	18B05-B07	1
Gehe	Clioquinol	22000908004	1
Gehe	Clioquinol	22000908008	1
GEHE	Clioquinol	22000908008	1
Gehe	Clioquinol	22000908012	1
Gehe	Clioquinol	22001088003	1
Gehe	Clioquinol	2208002-01	1
GEHE	Clioquinol	2208002-01	1
Gehe	Clioquinol	2300024003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Clioquinol	23000424007	1
Geibo/EuRho 16.09.2020	Clioquinol	1910030-01	1
Henry Lamote Oils GmbH	Clioquinol	28151-02562	1
Ichthyol-Gesellschaft	Clioquinol	1612020	1
Jenne	Clioquinol	2208002-01	1
Klenk	Clioquinol	11304120	1
L12	Clioquinol	1509038-03	2
L12	Clioquinol	1612020-01	2
M/s Eskayiodine Pvt....	Clioquinol	18278206	1
Nachprüfung	Clioquinol	13L26-N15	2
Nachprüfung	Clioquinol	3021U-02562	1
Nachprüfung	Clioquinol	AP200615-12	1
Noweda/Noweda	Clioquinol	16L18-B04-328520	1
Noweda/Noweda	Clioquinol	16L18-B04-329704	1
Noweda	Clioquinol	10057206	1
Noweda	Clioquinol	11304107	1
Noweda	Clioquinol	11304111	1
Noweda	Clioquinol	1201034-02	2
Noweda	Clioquinol	1309009-01	1
Noweda	Clioquinol	14359103	1
Noweda	Clioquinol	14359120	1
Noweda	Clioquinol	1612020-01	1
Noweda	Clioquinol	16307208	1
Noweda	Clioquinol	17204603	1
Noweda	Clioquinol	18278214	1
Noweda	Clioquinol	18278215	1
Noweda	Clioquinol	1903010-01	1
Noweda	Clioquinol	22000908003	1
Noweda	Clioquinol	22000908012	2
Noweda	Clioquinol	2208002-01	1
Noweda	Clioquinol	22G25-B03-222915	1
Noweda	Clioquinol	22G25-B03-227776	1
Phö/Dr.Wolff	Clioquinol	18011523	1
Phoenix	Clioquinol	11304119	1
Phoenix	Clioquinol	13114408	2
Phoenix	Clioquinol	13114417	1
Phoenix	Clioquinol	1612020-02	1
Phoenix	Clioquinol	16J18-B04-332852	2
Phoenix	Clioquinol	18011523	1
Phoenix	Clioquinol	18278206	1
Phoenix	Clioquinol	21000089001	2
Phoenix	Clioquinol	21000089006	2
Phoenix	Clioquinol	22000908008	1
Phoenix	Clioquinol	22001088003	1
Phoenix	Clioquinol	23000424001	1
Phoenix	Clioquinol	8178L17	1
Phönix Gotha	Clioquinol	11304124	1
phönix	Clioquinol		1
Phönix	Clioquinol	1102022-02	3
Phönix	Clioquinol	1201034-02	1
Phönix	Clioquinol	1309009-02	1
Phönix	Clioquinol	13114417	1
Phönix	Clioquinol	14C21-B06	2
Phönix	Clioquinol	14C21-B08	1
Phönix	Clioquinol	15L30-B05-314974	1
Phönix	Clioquinol	1612020-01	1
Phönix	Clioquinol	16718b04332852	1
Phönix	Clioquinol	182782008	1
Phönix	Clioquinol	1903010-01	1
Phönix	Clioquinol	1910030-02	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Clioquinol	2011013-01	1
Phönix	Clioquinol	21000089001	1
Phönix	Clioquinol	21000089006	1
Phönix	Clioquinol	22000908012	1
Phönix	Clioquinol	3165	1
Sanacorp	Clioquinol	11304111	1
Sanacorp	Clioquinol	11304124	1
Sanacorp	Clioquinol	1201034-01	1
Sanacorp	Clioquinol	13114422	1
Sanacorp	Clioquinol	1612020-03	1
Sanacorp	Clioquinol	16J18-B04-328511	1
Sanacorp	Clioquinol	1910030-01	1
Sanacorp	Clioquinol	20001561006	1
Sanacorp	Clioquinol	22000908004	1
Sanacorp	Clioquinol	22000908007	1
Sanacorp	Clioquinol	22G25-B03-227776	1
Sanacorp	Clioquinol	23000424001	1
Sanacorp	Clioquinol	8/AKD4	1
Sanacorp	Clioquinol	8075E19	1
Sanacorp04	Clioquinol	1612020-02	1
Synthexim / Gehe	Clioquinol	14359118	1
Synthexim	Clioquinol	1405080036	1
Unisan	Clioquinol	14/11-B03	1
VDL	Clioquinol	131144131	1
wepa/Sanaco	Clioquinol	1439118	1

- 234 076 spectra from 1515 *Apo-Ident* customers from a total of 48 907 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clioquinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clioquinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	570	0	201 514
Type C	0	1986	5	234 076

The substance/substance group *Clioquinol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9474 %)
Type C	100.0000 % (> 99.9007 %)	99.7489 % (> 99.5982 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20895	23047	6,68	203,70
21236	21246	6,35	202,77
21246	21246	0,00	201,17
21913	21944	6,42	198,87
21944	21944	0,00	198,43
21972	21246	9,46	197,28
23047	23047	0,00	202,38
27002	27002	0,00	179,27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloranfenicol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20097-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloranfenicol; Chloramphenicolum

Special notes

When selecting the *Cloranfenicol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloranfenicol	10	14	333

Second-stage model

For differentiation of the substance/substance group *Cloranfenicol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloranfenicol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	87,17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloranfenicol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloranfenicol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloranfenicol	11370716	20787	40	20120202
Caelo	Cloranfenicol	12248507	20807	40	20120831
Caelo	Cloranfenicol	13080924	21701	60	1509287
Caelo	Cloranfenicol	14346908	21988	60	20150115
Euro OTC	Cloranfenicol	1209019-02	20813	80	20130408
Euro OTC	Cloranfenicol	1209019-02	20815	80	20130408
Euro OTC	Cloranfenicol	1407043-01	21752	60	20140903
Euro OTC	Cloranfenicol	1602002	22367	45	20160309*
Fagron	Cloranfenicol	11F20-N05	20777	120	1412249
Fagron	Cloranfenicol	13A11-N02	20822	40	20130125
Fagron	Cloranfenicol	14E01-B02-308559	21910	60	20140513

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 685 spectra of 11 reference samples from the substance/substance group *Cloranfenicol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 277 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 610 spectra of 17 reference samples from the substance/substance group *Cloranfenicol*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloranfenicol	15358906	22961	40
Caelo	Cloranfenicol	162786	23353	40
Caelo	Cloranfenicol	180178	24049	40
Caelo	Cloranfenicol	192260	24892	40
Caelo	Cloranfenicol	20000261	25211	40
Caelo	Cloranfenicol	22002986	26495	40
Caelo	Cloranfenicol	24001644	27439	40
Euro OTC	Cloranfenicol	1704021	23392	40
Euro OTC	Cloranfenicol	1903028	24625	40
Euro OTC	Cloranfenicol	2002043	25264	40
Euro OTC	Cloranfenicol	2201014	25958	40
Euro OTC	Cloranfenicol	2306004	26924	40
Euro OTC	Cloranfenicol	2403008	27362	40
Fagron	Cloranfenicol	22B02-B09-219706	26158	40
Caelo	Cloranfenicol	22002986	26495SI	20
Euro OTC	Cloranfenicol	2201014	25958SI	10
Fagron	Cloranfenicol	22B02-B09-219706	26158SI	20

- 201 474 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3293 spectra from 977 *Apo-Ident* customers from 347 batches from the substance/substance group *Cloranfenicol*.

- Among them are spectra of independent samples from 330 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloranfenicol	2002043-03	1
	Cloranfenicol	21001144006	1
	Cloranfenicol	21001144009	1
	Cloranfenicol	21001144014	1
	Cloranfenicol	220002986002	1
	Cloranfenicol	22002986001	8
	Cloranfenicol	22002986002	2
	Cloranfenicol	22002986003	8
	Cloranfenicol	22002986006	2
	Cloranfenicol	22002986007	5
	Cloranfenicol	2201014-01	7
	Cloranfenicol	2201014-02	13
	Cloranfenicol	2201014-03	7
	Cloranfenicol	220101404	1
	Cloranfenicol	2201014-04	3
	Cloranfenicol	220104-02	1
	Cloranfenicol	221014-01	1
	Cloranfenicol	2306004-01	11
	Cloranfenicol	2306004-02	1
	Cloranfenicol	2403008-01	1
	Cloranfenicol	DY0092000082	1
4,64	Cloranfenicol	1903028-03	1
AHD	Cloranfenicol	12248507	1
AHD	Cloranfenicol	12248509	1
AHD	Cloranfenicol	13080904	1
AHD	Cloranfenicol	14346912	1
AHD	Cloranfenicol	18017807	1
AHD	Cloranfenicol	2306004-01	1
AHD	Cloranfenicol	2306004-02	2
AHDE 20.08.15	Cloranfenicol	DY00912128	1
Alliance 15.04.2015 ...	Cloranfenicol	1407043-01	1
Alliance Health	Cloranfenicol	1209019-02	1
Alliance Healthcare	Cloranfenicol	21001144009	1
Anzag 03.04.13 ek: 3,18EUR	Cloranfenicol	12248501	1
Anzag ek:2.98EUR 25.08.12	Cloranfenicol	11370711	1
Anzag	Cloranfenicol	1302024-01	1
Anzag	Cloranfenicol	1308017-02	1
ANZAG	Cloranfenicol	1308017-02	1
Anzag	Cloranfenicol	14346924	2
anzag	Cloranfenicol	15358907	1
Anzag	Cloranfenicol	1602002-03	1
apo-ident	Cloranfenicol	1602002-03	1
Audor Pharma	Cloranfenicol	2002043/01	1
Audor Pharma	Cloranfenicol	2201014-01	1
Beiersdorf	Cloranfenicol	1704021-03	1
Bombastus	Cloranfenicol	1308017-01	1
Bombastus	Cloranfenicol	1602002-03	1
Bombastus	Cloranfenicol	1704021-01	1
Bombastus	Cloranfenicol	2002043-01	3
Caelo	Cloranfenicol		1
Caelo	Cloranfenicol	10341703	1
Caelo	Cloranfenicol	10341707	1
Caelo	Cloranfenicol	10341711	2
Caelo	Cloranfenicol	10341717	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloranfenicol	1062002-04	1
Caelo	Cloranfenicol	11031402	1
Caelo	Cloranfenicol	1137004	1
Caelo	Cloranfenicol	1137070	1
Caelo	Cloranfenicol	11370702	3
Caelo	Cloranfenicol	11370703	2
Caelo	Cloranfenicol	11370705	3
Caelo	Cloranfenicol	11370706	3
Caelo	Cloranfenicol	11370707	2
Caelo	Cloranfenicol	11370711	12
Caelo	Cloranfenicol	11370712	4
Caelo	Cloranfenicol	11370713	3
Caelo	Cloranfenicol	11370714	2
Caelo	Cloranfenicol	11370715	1
Caelo	Cloranfenicol	11370716	4
Caelo	Cloranfenicol	11370717	2
Caelo	Cloranfenicol	1137714	1
Caelo	Cloranfenicol	1203012-02	1
Caelo	Cloranfenicol	12072606	1
Caelo	Cloranfenicol	12248501	12
Caelo	Cloranfenicol	12248505	2
Caelo	Cloranfenicol	12248506	8
Caelo	Cloranfenicol	12248507	9
Caelo	Cloranfenicol	12248509	12
Caelo	Cloranfenicol	12248520	7
Caelo	Cloranfenicol	12248524	7
Caelo	Cloranfenicol	12248525	7
Caelo	Cloranfenicol	12g02n01	1
Caelo	Cloranfenicol	12G02-N01	2
Caelo	Cloranfenicol	1302024-01	1
Caelo	Cloranfenicol	1302024-02	2
Caelo	Cloranfenicol	130416-1	1
Caelo	Cloranfenicol	130416-2	1
Caelo	Cloranfenicol	1308017-01	1
Caelo	Cloranfenicol	13080303	1
Caelo	Cloranfenicol	130809	1
Caelo	Cloranfenicol	13080902	1
Caelo	Cloranfenicol	13080903	8
Caelo	Cloranfenicol	13080904	5
Caelo	Cloranfenicol	13080907	13
Caelo	Cloranfenicol	13080908	4
Caelo	Cloranfenicol	13080915	1
Caelo	Cloranfenicol	13080917	4
Caelo	Cloranfenicol	13080918	2
Caelo	Cloranfenicol	13080921	4
Caelo	Cloranfenicol	13080923	13
Caelo	Cloranfenicol	13080924	15
Caelo	Cloranfenicol	13080925	11
Caelo	Cloranfenicol	13A31-B02	1
Caelo	Cloranfenicol	13A31-B02-286709	1
Caelo	Cloranfenicol	140704301	2
Caelo	Cloranfenicol	1407043-01	1
Caelo	Cloranfenicol	14246917	1
Caelo	Cloranfenicol	1434608	1
Caelo	Cloranfenicol	14346901	2
Caelo	Cloranfenicol	14346903	1
Caelo	Cloranfenicol	14346904	4
Caelo	Cloranfenicol	14346906	4
Caelo	Cloranfenicol	14346907	9
Caelo	Cloranfenicol	14346908	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloranfenicol	14346910	15
Caelo	Cloranfenicol	14346911	22
Caelo	Cloranfenicol	14346912	3
Caelo	Cloranfenicol	14346913	8
Caelo	Cloranfenicol	14346914	4
Caelo	Cloranfenicol	14346917	8
Caelo	Cloranfenicol	14346918	18
Caelo	Cloranfenicol	14346918I-080816-1	1
Caelo	Cloranfenicol	14346922	1
Caelo	Cloranfenicol	14346924	5
Caelo	Cloranfenicol	14356910	1
Caelo	Cloranfenicol	1436908	1
Caelo	Cloranfenicol	1436918	1
Caelo	Cloranfenicol	14E01-B02-296623	1
Caelo	Cloranfenicol	14E01B02296624	1
Caelo	Cloranfenicol	14E01-B02-308559	2
Caelo	Cloranfenicol	14E001-B02	1
Caelo	Cloranfenicol	1502036-01	3
Caelo	Cloranfenicol	1502036-02	2
Caelo	Cloranfenicol	150203603	1
Caelo	Cloranfenicol	1502036-03	4
Caelo	Cloranfenicol	150528C	1
Caelo	Cloranfenicol	153589	1
Caelo	Cloranfenicol	15358903	3
Caelo	Cloranfenicol	15358905	25
Caelo	Cloranfenicol	15358906	13
Caelo	Cloranfenicol	15358907	3
Caelo	Cloranfenicol	15358908	10
Caelo	Cloranfenicol	15358909	6
Caelo	Cloranfenicol	15358911	1
Caelo	Cloranfenicol	15358912	14
Caelo	Cloranfenicol	15358913	28
Caelo	Cloranfenicol	15358914	21
Caelo	Cloranfenicol	1535896	1
Caelo	Cloranfenicol	160200201	1
Caelo	Cloranfenicol	1602002-01	5
Caelo	Cloranfenicol	1602002-02	2
Caelo	Cloranfenicol	1602002-03	1
Caelo	Cloranfenicol	16258612	1
Caelo	Cloranfenicol	16278009	1
Caelo	Cloranfenicol	16278601	1
Caelo	Cloranfenicol	16278602	9
Caelo	Cloranfenicol	16278605	1
Caelo	Cloranfenicol	16278606	12
Caelo	Cloranfenicol	16278608	18
Caelo	Cloranfenicol	16278609	29
Caelo	Cloranfenicol	16278609/180420CA	1
Caelo	Cloranfenicol	16278610	1
Caelo	Cloranfenicol	16278611	2
Caelo	Cloranfenicol	16278612	31
Caelo	Cloranfenicol	1627862	1
Caelo	Cloranfenicol	1627898	1
Caelo	Cloranfenicol	16358909	1
Caelo	Cloranfenicol	170402101	1
Caelo	Cloranfenicol	1704021-01	18
Caelo	Cloranfenicol	1704021-02	7
Caelo	Cloranfenicol	1704021-03	3
Caelo	Cloranfenicol	1704021-04	8
Caelo	Cloranfenicol	17343802	13
Caelo	Cloranfenicol	17343803	32

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloranfenicol	174021-02	2
Caelo	Cloranfenicol	180178	1
Caelo	Cloranfenicol	18017802	6
Caelo	Cloranfenicol	18017804	5
Caelo	Cloranfenicol	18017806	40
Caelo	Cloranfenicol	18017807	14
Caelo	Cloranfenicol	18017809	37
Caelo	Cloranfenicol	18017810	9
Caelo	Cloranfenicol	18017811	22
Caelo	Cloranfenicol	18017813	4
Caelo	Cloranfenicol	18017814	9
Caelo	Cloranfenicol	18025702	2
Caelo	Cloranfenicol	181017809	1
Caelo	Cloranfenicol	1903028-01	10
Caelo	Cloranfenicol	1903028-02	6
Caelo	Cloranfenicol	1903028-041	1
Caelo	Cloranfenicol	19222226003	1
Caelo	Cloranfenicol	19225003	1
Caelo	Cloranfenicol	192260001	3
Caelo	Cloranfenicol	19226001	1
Caelo	Cloranfenicol	19226002	25
Caelo	Cloranfenicol	19226003	99
Caelo	Cloranfenicol	19226003P-200323-1	1
Caelo	Cloranfenicol	19226004	1
Caelo	Cloranfenicol	1922603	1
Caelo	Cloranfenicol	20000261003	8
Caelo	Cloranfenicol	20000261004	37
Caelo	Cloranfenicol	20003760002	12
Caelo	Cloranfenicol	20003760003	55
Caelo	Cloranfenicol	20003760006	5
Caelo	Cloranfenicol	2000376003	1
Caelo	Cloranfenicol	2000376006	1
Caelo	Cloranfenicol	2002043-01	4
Caelo	Cloranfenicol	2002043-02	4
Caelo	Cloranfenicol	200204303	1
Caelo	Cloranfenicol	2003760003	2
Caelo	Cloranfenicol	20102012J1	1
Caelo	Cloranfenicol	21001144003	3
Caelo	Cloranfenicol	21001144004	21
Caelo	Cloranfenicol	21001144006	6
Caelo	Cloranfenicol	21001144007	17
Caelo	Cloranfenicol	21001144010	1
Caelo	Cloranfenicol	21001144014	2
Caelo	Cloranfenicol	2100144004	2
Caelo	Cloranfenicol	21002415002	1
Caelo	Cloranfenicol	2181116	1
Caelo	Cloranfenicol	22002986001	3
Caelo	Cloranfenicol	22002986003	3
Caelo	Cloranfenicol	2201014-01	5
Caelo	Cloranfenicol	28011401	1
Caelo	Cloranfenicol	3081602	1
Caelo	Cloranfenicol	310311	1
Caelo	Cloranfenicol	3125204	1
Caelo	Cloranfenicol	3217A-01259	1
Caelo	Cloranfenicol	4412Q-01259	1
Caelo	Cloranfenicol	4654572	1
Caelo	Cloranfenicol	4712Q-01259	1
Caelo	Cloranfenicol	8017811	1
Caelo	Cloranfenicol	82853399	1
Caelo	Cloranfenicol	8701	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloranfenicol	93323801	1
Caelo	Cloranfenicol	DY00911233	1
Caelo	Cloranfenicol	DY00916161	1
Caelo	Cloranfenicol	DY130525	2
Caeol/Noweda	Cloranfenicol	19226003	2
Caeolo / Anzag	Cloranfenicol	15358914	1
Caeolo	Cloranfenicol	20003760003	4
Caesar & Loretz Gmb	Cloranfenicol	18017814	2
Caesar & Loretz GmbH...	Cloranfenicol	19226003	2
Caesar & Loretz GmbH...	Cloranfenicol	18017809	1
Caesar & Loretz GmbH...	Cloranfenicol	18017811	1
Caesar & Loretz GmbH...	Cloranfenicol	20000261004	1
Caesar & Loretz GmbH...	Cloranfenicol	21001144004	2
Caesar & Loretz GmbH...	Cloranfenicol	20003760002	1
Caesar & Loretz GmbH...	Cloranfenicol	21001144004	1
Caesar & Loretz GmbH...	Cloranfenicol	22002986001	1
Caesar & Loretz GmbH...	Cloranfenicol	19226003	1
Caesar & Loretz GmbH...	Cloranfenicol	20000261003	1
Caesar & Loretz GmbH...	Cloranfenicol	20003760002	1
Caesar & Loretz GmbH...	Cloranfenicol	19226003	1
Caesar & Loretz GmbH...	Cloranfenicol	21001144007	2
Caesar & Loretz GmbH...	Cloranfenicol	21001144004	1
Caesar & Loretz GmbH...	Cloranfenicol	18017809	1
Caesar & Loretz GmbH...	Cloranfenicol	20003760003	3
Caesar & Loretz GmbH/Gehe	Cloranfenicol	18017811	2
Caesar & Loretz GmbH/Gehe	Cloranfenicol	20003760002	1
Caesar & Loretz GmbH/Gehe	Cloranfenicol	21001144007	1
Caesar & Loretz GmbH...	Cloranfenicol	20003760003	1
Caesar & Loretz GmbH...	Cloranfenicol	19226002	1
Caesar & Loretz GmbH...	Cloranfenicol	20000261004	1
Caesar & Loretz GmbH...	Cloranfenicol	20003760003	1
Caesar & Loretz GmbH...	Cloranfenicol	192260001	1
Caesar & Loretz GmbH/Otto	Cloranfenicol	19226003	1
Caesar & Loretz GmbH...	Cloranfenicol	18017814	1
Caesar & Loretz GmbH...	Cloranfenicol	20000261004	1
Caesar & Loretz GmbH...	Cloranfenicol	20003760003	3
Caesar & Loretz GmbH...	Cloranfenicol	20000261004	2
Caesar & Loretz GmbH...	Cloranfenicol	20003760003	1
Caesar & Loretz GmbH...	Cloranfenicol	21001144004	1
Caesar & Loretz GmbH...	Cloranfenicol	18017811	1
Caesar & Loretz GmbH	Cloranfenicol	11370711	1
Caesar & Loretz GmbH	Cloranfenicol	18017806	1
Caesar & Loretz GmbH	Cloranfenicol	18017809	6
Caesar & Loretz GmbH	Cloranfenicol	18017810	2
Caesar & Loretz GmbH	Cloranfenicol	18017811	8
Caesar & Loretz GmbH	Cloranfenicol	18017813	1
Caesar & Loretz GmbH	Cloranfenicol	18017814	3
Caesar & Loretz GmbH	Cloranfenicol	1903028-01	1
Caesar & Loretz GmbH	Cloranfenicol	1903028-02	3
Caesar & Loretz GmbH	Cloranfenicol	192260001	1
Caesar & Loretz GmbH	Cloranfenicol	19226001	1
Caesar & Loretz GmbH	Cloranfenicol	19226002	12
Caesar & Loretz GmbH	Cloranfenicol	19226003	57
Caesar & Loretz GmbH	Cloranfenicol	19226004	2
Caesar & Loretz GmbH	Cloranfenicol	20000261003	3
Caesar & Loretz GmbH	Cloranfenicol	20000261004	9
Caesar & Loretz GmbH	Cloranfenicol	20003343004	1
Caesar & Loretz GmbH	Cloranfenicol	20003760002	5
Caesar & Loretz GmbH	Cloranfenicol	20003760003	28
Caesar & Loretz GmbH	Cloranfenicol	20003760006	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloranfenicol	2000376003	1
Caesar & Loretz GmbH	Cloranfenicol	21001144004	18
Caesar & Loretz GmbH	Cloranfenicol	21001144006	2
Caesar & Loretz GmbH	Cloranfenicol	21001144007	11
Caesar & Loretz GmbH	Cloranfenicol	21001144009	1
Caesar & Loretz GmbH	Cloranfenicol	21001144014	2
Caesar & Loretz GmbH	Cloranfenicol	22002986001	2
Caesar & Loretz	Cloranfenicol	15358908	1
Caesar & Loretz	Cloranfenicol	16278609	2
Caesar & Loretz	Cloranfenicol	18017809	1
Caesar & Loretz	Cloranfenicol	21001144004	1
Caesar & Loretz	Cloranfenicol	21001144014	1
Caesar&Lorenz	Cloranfenicol	20003760003	1
Caesar&Loretz	Cloranfenicol	16278612	1
Caeser und Loretz GmbH	Cloranfenicol	19226002	1
Caleo/ Noweda	Cloranfenicol	173436803	1
Caolo- Noweda	Cloranfenicol	14346908	1
Cealo/Gehe	Cloranfenicol	2100114406	3
Cealo	Cloranfenicol	1602002-03	1
Chloramphenicol	Cloranfenicol	2002043-01	1
Eu Rho Pharm/E	Cloranfenicol	1903028-02	1
Eu Rho Pharm/K	Cloranfenicol	1704021-04	1
Eur Rho Phönix	Cloranfenicol	2002043-02	1
EuRho / 20	Cloranfenicol	1502036-01	1
EuRho / Noweda	Cloranfenicol	1903028-02	1
Eurho No	Cloranfenicol	1903028-01	1
EuRho Noweda	Cloranfenicol	2002043-01	1
Eurho ph	Cloranfenicol	1903028-02	1
Eurho Phönix	Cloranfenicol	1704021-02	1
Eurho Phönix	Cloranfenicol	2002043-02	2
EuRho/ Phönix	Cloranfenicol	1704021-01	2
EuRho/ Phönix	Cloranfenicol	20002043-01	1
EuRho/ Sanacorp	Cloranfenicol	2002043-02	1
Eurho/AHD	Cloranfenicol	2002043-02	1
EuRho/Alliance	Cloranfenicol	2002043-01	1
EuRho/Gehe	Cloranfenicol	1704021-04	1
EuRho/Gehe	Cloranfenicol	1903028-02	1
EuRho/Gehe	Cloranfenicol	2002043-01	1
EuRho/Gehe	Cloranfenicol	919110016	1
EuRho/Noweda	Cloranfenicol	1704021-02	1
EuRho/Noweda	Cloranfenicol	2002043-02	1
EuRho/Phoenix	Cloranfenicol	2002043-01	3
EuRho/Phoenix	Cloranfenicol	2201014-03	1
EuRho/Phönix	Cloranfenicol	123012-01	1
EuRho/Phönix	Cloranfenicol	1308017-01	1
EuRho/Phönix	Cloranfenicol	1903028-02	1
Eurho/Phönix	Cloranfenicol	2002043-01	1
EuRho/Phönix	Cloranfenicol	2002043-01	1
EuRho/Sanacorp	Cloranfenicol	1704021-01	1
EuRho/Sanacorp	Cloranfenicol	2002043-03	2
EuRho	Cloranfenicol	1308017-02	1
EuRho	Cloranfenicol	15358913	1
EuRho	Cloranfenicol	1704021-01	2
EuRho	Cloranfenicol	1704021-02	2
EuRho	Cloranfenicol	1704021-03	2
EuRho	Cloranfenicol	1704021-04	1
Eurho	Cloranfenicol	1704087-03	1
EuRho	Cloranfenicol	1903028-01	2
Eurho	Cloranfenicol	1903028-02	1
EuRho	Cloranfenicol	1903028-02	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Cloranfenicol	2002043-01	4
EuRho	Cloranfenicol	2002043-02	3
euRho	Cloranfenicol	2002043-03	2
Eurho	Cloranfenicol	2002043-03	1
EuRho	Cloranfenicol	2002043-03	2
EuRho	Cloranfenicol	2002043-1	1
EuRho	Cloranfenicol	216A-01259	1
Euro OCT / Krieger	Cloranfenicol	2002043-01	1
Euro OCT	Cloranfenicol	1203012-02	1
Euro OTC	Cloranfenicol		5
Euro OTC	Cloranfenicol	10061707	1
Euro OTC	Cloranfenicol	1012013-01	2
Euro OTC	Cloranfenicol	1107002-01	2
Euro OTC	Cloranfenicol	110700202	1
Euro OTC	Cloranfenicol	1107002-02	1
Euro OTC	Cloranfenicol	120250	1
Euro OTC	Cloranfenicol	1203012-01	7
Euro OTC	Cloranfenicol	1203012-02	12
Euro OTC	Cloranfenicol	1203012-12	1
Euro OTC	Cloranfenicol	1209010-02	3
Euro OTC	Cloranfenicol	1209019-01	6
Euro OTC	Cloranfenicol	120901902	3
Euro OTC	Cloranfenicol	1209019-02	11
Euro OTC	Cloranfenicol	1302024-01	12
Euro OTC	Cloranfenicol	1302024-02	7
Euro OTC	Cloranfenicol	130801701	1
Euro OTC	Cloranfenicol	1308017-01	10
Euro OTC	Cloranfenicol	130801702	2
Euro OTC	Cloranfenicol	1308017-02	11
Euro OTC	Cloranfenicol	13111410	1
Euro OTC	Cloranfenicol	1317M-01259	1
Euro OTC	Cloranfenicol	1407043	1
Euro OTC	Cloranfenicol	140704301	5
Euro OTC	Cloranfenicol	1407043-01	24
Euro OTC	Cloranfenicol	14101717	1
Euro OTC	Cloranfenicol	14346910	1
Euro OTC	Cloranfenicol	1502036	1
Euro OTC	Cloranfenicol	150203601	5
Euro OTC	Cloranfenicol	1502036-01	34
Euro OTC	Cloranfenicol	150203602	2
Euro OTC	Cloranfenicol	1502036-02	19
Euro OTC	Cloranfenicol	1502036022016030911	1
Euro OTC	Cloranfenicol	150203603	1
Euro OTC	Cloranfenicol	1502036-03	23
Euro OTC	Cloranfenicol	1502063-02	1
Euro OTC	Cloranfenicol	1509211259	1
Euro OTC	Cloranfenicol	15358906	1
Euro OTC	Cloranfenicol	15358914	4
Euro OTC	Cloranfenicol	16020002-02	1
Euro OTC	Cloranfenicol	16020002-03	1
Euro OTC	Cloranfenicol	1602002-01	43
Euro OTC	Cloranfenicol	1602002-02	28
Euro OTC	Cloranfenicol	160200203	2
Euro OTC	Cloranfenicol	1602002-03	41
Euro OTC	Cloranfenicol	1602002-04	2
Euro OTC	Cloranfenicol	1602002-07	1
Euro OTC	Cloranfenicol	1701021-04	1
Euro OTC	Cloranfenicol	1704021	4
Euro OTC	Cloranfenicol	1704021_02	1
Euro OTC	Cloranfenicol	170402101	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloranfenicol	1704021-01	102
Euro OTC	Cloranfenicol	1704021-015505	1
Euro OTC	Cloranfenicol	1704021-01A	1
Euro OTC	Cloranfenicol	170402102	1
Euro OTC	Cloranfenicol	1704021-02	58
Euro OTC	Cloranfenicol	170402103	3
Euro OTC	Cloranfenicol	1704021-03	50
Euro OTC	Cloranfenicol	170402104	2
Euro OTC	Cloranfenicol	1704021-04	73
Euro OTC	Cloranfenicol	17040212-04	1
Euro OTC	Cloranfenicol	170421-01	1
Euro OTC	Cloranfenicol	17044021-01	1
Euro OTC	Cloranfenicol	1707021-02	1
Euro OTC	Cloranfenicol	17704021-01	1
Euro OTC	Cloranfenicol	18017802	1
Euro OTC	Cloranfenicol	18017809	2
Euro OTC	Cloranfenicol	180178091903028-01	1
Euro OTC	Cloranfenicol	1903028	7
Euro OTC	Cloranfenicol	1903028_01	1
Euro OTC	Cloranfenicol	190302801	6
Euro OTC	Cloranfenicol	1903028-01	128
Euro OTC	Cloranfenicol	1903028-010	1
Euro OTC	Cloranfenicol	190302802	1
Euro OTC	Cloranfenicol	1903028-02	105
Euro OTC	Cloranfenicol	190302803	1
Euro OTC	Cloranfenicol	1903028-03	30
Euro OTC	Cloranfenicol	1903028-42	1
Euro OTC	Cloranfenicol	191210111	1
Euro OTC	Cloranfenicol	193028-03	1
Euro OTC	Cloranfenicol	20012043-02	1
Euro OTC	Cloranfenicol	2002043	3
Euro OTC	Cloranfenicol	200204301	2
Euro OTC	Cloranfenicol	2002043-01	102
Euro OTC	Cloranfenicol	2002043-01/4420	1
Euro OTC	Cloranfenicol	200204302	5
Euro OTC	Cloranfenicol	2002043-02	142
Euro OTC	Cloranfenicol	200204303	4
Euro OTC	Cloranfenicol	2002043-03	45
Euro OTC	Cloranfenicol	2002043-1	1
Euro OTC	Cloranfenicol	20022043-01	1
Euro OTC	Cloranfenicol	200243-02	2
Euro OTC	Cloranfenicol	2004030-01	1
Euro OTC	Cloranfenicol	211217(2002043-01)	1
Euro OTC	Cloranfenicol	2121211203012-0	1
Euro OTC	Cloranfenicol	2201014-01	31
Euro OTC	Cloranfenicol	2201014-02	10
Euro OTC	Cloranfenicol	2201014-04	2
Euro OTC	Cloranfenicol	22010144-01	1
Euro OTC	Cloranfenicol	221014-02	1
Euro OTC	Cloranfenicol	2306004-01	1
Euro OTC	Cloranfenicol	314Q1259	1
Euro OTC	Cloranfenicol	90302801	1
Euro OTC	Cloranfenicol	916161	1
Euro OTC	Cloranfenicol	919110016	6
Euro OTC	Cloranfenicol	DY00912128	6
Euro OTC	Cloranfenicol	DY00914151	1
Euro OTC	Cloranfenicol	DY00918024	1
Euro OTC	Cloranfenicol	DY00918024/1903028-02	1
Euro OTC	Cloranfenicol	DY0092000082	2
Euro OTC	Cloranfenicol	DY130525	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloranfenicol	T02-55/1407043-01	1
Euro OTG	Cloranfenicol	1502036-01	1
euro pharm	Cloranfenicol	1602002-01	1
Euro/ Sanacorp	Cloranfenicol	1308017-02	1
Euro//Sanacorp	Cloranfenicol	2002043-01	1
EUro/AHD	Cloranfenicol	1209019-01	1
EUro/AHD	Cloranfenicol	1209019-02	1
Euro/Alliance Healthcare	Cloranfenicol	1502036-01	1
Euro/Krieger	Cloranfenicol	1602002-02	1
Euro/Krieger	Cloranfenicol	1602002-03	1
Euro/Noweda	Cloranfenicol	1602002-02	1
Euro/Phönix	Cloranfenicol	1502036-03	1
Euro/Phönix	Cloranfenicol	1704021-02	1
Euro/Phönix	Cloranfenicol	1704021-04	1
Euro/Phönix	Cloranfenicol	1903028-01	1
euro	Cloranfenicol	2002043-01	1
EurPS	Cloranfenicol	1502036-01	2
Fagron	Cloranfenicol		2
Fagron	Cloranfenicol	11/14-N03	2
Fagron	Cloranfenicol	11J14-N03	1
Fagron	Cloranfenicol	120250-0002	1
Fagron	Cloranfenicol	1202500003	1
Fagron	Cloranfenicol	12A11-N02	1
Fagron	Cloranfenicol	12B13-N06	6
Fagron	Cloranfenicol	12F01-N23	1
Fagron	Cloranfenicol	12G02-N01	9
Fagron	Cloranfenicol	12L11-N06	9
Fagron	Cloranfenicol	13A11N02	1
Fagron	Cloranfenicol	13A11-N02	6
Fagron	Cloranfenicol	13A31-B02	8
Fagron	Cloranfenicol	13A31-B02_286708	1
Fagron	Cloranfenicol	13A31-B02-286708	4
Fagron	Cloranfenicol	13A31-B02-286709	2
Fagron	Cloranfenicol	13A31-B02-290263	1
Fagron	Cloranfenicol	13A31-B02-290300	4
Fagron	Cloranfenicol	14E01-B02	5
Fagron	Cloranfenicol	14E01-B02_296624	1
Fagron	Cloranfenicol	14E01-B02-296623	1
Fagron	Cloranfenicol	14e01-b02-296624	1
Fagron	Cloranfenicol	14E01B02296624	2
Fagron	Cloranfenicol	14E01-B02-296624	7
Fagron	Cloranfenicol	14E01-B02-296625	1
Fagron	Cloranfenicol	14E01-B02-306146	7
Fagron	Cloranfenicol	14E01-B02-308559	7
Fagron	Cloranfenicol	1502036-01	1
Fagron	Cloranfenicol	15358914	1
Fagron	Cloranfenicol	1602002-01	2
Fagron	Cloranfenicol	1602002-02	1
Fagron	Cloranfenicol	1602002-03	1
Fagron	Cloranfenicol	1612-B07-329313	1
Fagron	Cloranfenicol	1704021-01	1
Fagron	Cloranfenicol	1903028-01	1
Fagron	Cloranfenicol	1903028-02	1
Fagron	Cloranfenicol	2002043-01	2
Fagron	Cloranfenicol	20E14-B19-202352	2
Fagron	Cloranfenicol	2111I-01259	1
Fagron	Cloranfenicol	DY00911233	4
Fagron	Cloranfenicol	DY00912129	1
Fagron	Cloranfenicol	LTOCHL/049/16-17M	1
Fiebig	Cloranfenicol	1502036-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Cloranfenicol	15358913	1
Fiebig	Cloranfenicol	1602002-01	1
Fiebig	Cloranfenicol	16278608	1
Fiebig	Cloranfenicol	16278609	1
Fiebig	Cloranfenicol	16278612	1
Fiebig	Cloranfenicol	1704021-01	1
Fiebig	Cloranfenicol	1734803	1
Fiebig	Cloranfenicol	18017809	1
Fiebig	Cloranfenicol	18017810	1
Fiebig	Cloranfenicol	19226002	1
Finteler Apotheke	Cloranfenicol	15358913	1
Fischar/Sanacorp	Cloranfenicol	1704021-04	1
Fischer/ Noweda	Cloranfenicol	1502036-03	1
Fragon	Cloranfenicol	12G02-N01	1
Gatt-Koller / Phoenix	Cloranfenicol	5615/12115211	1
Gehe - Hedinger	Cloranfenicol	1704021-01	1
Gehe 27.06.15/euro	Cloranfenicol	1502036-01	2
Gehe amax	Cloranfenicol	1602002-03	1
gehe/ Northeast Pharma	Cloranfenicol	2002043-01	1
Gehe	Cloranfenicol	1107002-02	1
Gehe	Cloranfenicol	1203012-01	1
Gehe	Cloranfenicol	1209019-02	1
Gehe	Cloranfenicol	1308017-02	1
Gehe	Cloranfenicol	14346910	1
Gehe	Cloranfenicol	15358906	1
Gehe	Cloranfenicol	15358909	1
Gehe	Cloranfenicol	15358913	2
GEHE	Cloranfenicol	15358914	1
GEHE	Cloranfenicol	160200202	1
GEHE	Cloranfenicol	16278608	1
Gehe	Cloranfenicol	16278612	1
Gehe	Cloranfenicol	17021-04	1
Gehe	Cloranfenicol	1704021-01	3
Gehe	Cloranfenicol	1704021-02	3
Gehe	Cloranfenicol	1704021-03	2
Gehe	Cloranfenicol	1704021-04	1
GEHE	Cloranfenicol	17343803	1
GEHE	Cloranfenicol	18017806	1
Gehe	Cloranfenicol	18017811	1
GEHE	Cloranfenicol	18017811	1
Gehe	Cloranfenicol	1903028_02	1
Gehe	Cloranfenicol	1903028-01	6
Gehe	Cloranfenicol	1903028-02	1
Gehe	Cloranfenicol	1903028-03	1
GEHE	Cloranfenicol	19226002	1
Gehe	Cloranfenicol	19226003	1
Gehe	Cloranfenicol	2002043-01	1
Gehe	Cloranfenicol	2002043-02	1
Gehe	Cloranfenicol	22002986007	1
Gehe	Cloranfenicol	2201014-01	1
GEHE	Cloranfenicol	2201014-02	1
GEHE	Cloranfenicol	2201014-03	1
Gutenberg-Apotheke	Cloranfenicol	13A31-B02-286710	1
Jenne	Cloranfenicol	1903028	1
Jenne	Cloranfenicol	200204301	1
Jenne	Cloranfenicol	2002043-02	1
Kehr	Cloranfenicol	1704021-01	1
Kehr	Cloranfenicol	22002986001	1
Kehr	Cloranfenicol	22005298	1
Kehr	Cloranfenicol	2200986001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Mehta API	Cloranfenicol	181113082	1
Nanjing / Gehe	Cloranfenicol	14346910	1
Nanjing Baijingyu Ph...	Cloranfenicol	14346917	1
Nanjing Baijingyu Ph...	Cloranfenicol	13080908	2
NanjingBajingyu	Cloranfenicol	1538914	1
Northeast Gen	Cloranfenicol	DY122127	1
Northeast General / Gehe	Cloranfenicol	1602002-02	1
Northeast General/Noweda	Cloranfenicol	1502036-02	1
Northeast General	Cloranfenicol	1407043-01	1
Northeast General	Cloranfenicol	1602002-02	1
Northeast General	Cloranfenicol	1704021-01	2
Northeast General	Cloranfenicol	DY00914151	2
Northeast/Noweda	Cloranfenicol	DY00918024	1
Noweda/EuRho	Cloranfenicol	2002043-01	1
Noweda	Cloranfenicol	1137014	1
Noweda	Cloranfenicol	11370712	1
Noweda	Cloranfenicol	12248509	1
noweda	Cloranfenicol	13080908	2
Noweda	Cloranfenicol	14346901	2
Noweda	Cloranfenicol	14346910	1
Noweda	Cloranfenicol	1502036-03	1
Noweda	Cloranfenicol	15358906	1
Noweda	Cloranfenicol	15358914	1
Noweda	Cloranfenicol	1602002-02	1
Noweda	Cloranfenicol	16278609	1
Noweda	Cloranfenicol	1704021-01	3
Noweda	Cloranfenicol	1704021-02	2
Noweda	Cloranfenicol	1903028	2
Noweda	Cloranfenicol	1903028-01	1
Noweda	Cloranfenicol	1903028-02	1
Noweda	Cloranfenicol	192260001	1
Noweda	Cloranfenicol	19226002	1
Noweda	Cloranfenicol	2002043-02	1
noweda	Cloranfenicol	22002986002	1
Noweda	Cloranfenicol	22002986002	1
Noweda	Cloranfenicol	22002986003	1
NOWEDA	Cloranfenicol	22002986003	1
Noweda	Cloranfenicol	2201014-02	3
Noweda	Cloranfenicol	2201014-04	1
Noweda	Cloranfenicol	220104-01	1
Noweda	Cloranfenicol	2202986003	1
Parthe Apotheke	Cloranfenicol	67/20	1
Ph/Euro	Cloranfenicol	1704021-02	1
Ph/Euro	Cloranfenicol	2002043-03	1
Phoe	Cloranfenicol	15358905	1
PHOENIX 25.04.2014	Cloranfenicol	1308017-02	2
Phoenix	Cloranfenicol	13080903	1
Phoenix	Cloranfenicol	16278609	1
Phoenix	Cloranfenicol	1704021-01	1
phoenix	Cloranfenicol	1704021-02	1
Phoenix	Cloranfenicol	1704021-02	1
Phoenix	Cloranfenicol	18017814	1
phoenix	Cloranfenicol	1903028	1
Phoenix	Cloranfenicol	1903028-01	2
Phoenix	Cloranfenicol	2002043	1
Phoenix	Cloranfenicol	2002043-01	1
Phoenix	Cloranfenicol	200204302	1
Phoenix	Cloranfenicol	2002043-02	1
Phoenix	Cloranfenicol	22002986007	1
Phoenix	Cloranfenicol	2201014-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Cloranfenicol	2306004-01	1
Phoenix	Cloranfenicol	3087	1
phoenix-06.11.18	Cloranfenicol	17343803	1
Phönix /EURO	Cloranfenicol	2002043-01	1
Phönix 11.11.2019	Cloranfenicol	19226003	1
Phönix 12.10.2019	Cloranfenicol	1903028-01	1
Phönix Gotha	Cloranfenicol	13080907	1
Phönix/Fagon	Cloranfenicol	14346922	1
Phönix	Cloranfenicol	10341710	1
Phönix	Cloranfenicol	10341716	1
Phönix	Cloranfenicol	13080921	1
Phönix	Cloranfenicol	13A11-N02	3
Phönix	Cloranfenicol	13A1-802	3
phönix	Cloranfenicol	15358912	1
PHÖNIX	Cloranfenicol	16278608	1
Phönix	Cloranfenicol	170402103	1
Phönix	Cloranfenicol	18017806	1
Phönix	Cloranfenicol	1903028	1
Phönix	Cloranfenicol	1903028-02	1
Phönix	Cloranfenicol	190328-03	1
Phönix	Cloranfenicol	20003760003	1
Phönix	Cloranfenicol	2002043-01	4
Phönix	Cloranfenicol	2002043-02	2
Phönix	Cloranfenicol	22002986007	3
Phönix	Cloranfenicol	3157	1
Sana 22.11.2017 5.90	Cloranfenicol	16278608	1
Sanacorp 26.09.19 Ek…	Cloranfenicol	1903028-01	2
Sanacorp/EuRho	Cloranfenicol	1704021-02	1
Sanacorp	Cloranfenicol		1
Sanacorp	Cloranfenicol	11370711	1
Sanacorp	Cloranfenicol	120901902	1
Sanacorp	Cloranfenicol	12248501	1
Sanacorp	Cloranfenicol	1308017-02	1
Sanacorp	Cloranfenicol	140704301	1
Sanacorp	Cloranfenicol	1407043-01	2
Sanacorp	Cloranfenicol	1502036-01	1
Sanacorp	Cloranfenicol	15358913	1
Sanacorp	Cloranfenicol	16278612	1
Sanacorp	Cloranfenicol	1704021-01	1
Sanacorp	Cloranfenicol	17343803	1
Sanacorp	Cloranfenicol	18017806	2
Sanacorp	Cloranfenicol	18017809	1
Sanacorp	Cloranfenicol	18017814	2
Sanacorp	Cloranfenicol	1903028-02	2
Sanacorp	Cloranfenicol	19226003	1
Sanacorp	Cloranfenicol	21001144004	1
Sanacorp	Cloranfenicol	22002986001	2
Sanacorp	Cloranfenicol	220101-04	1
Sanacorp	Cloranfenicol	2201014-01	1
sanacorp	Cloranfenicol	2201014-04	1
Sanacorp	Cloranfenicol	2306004-01	1
Sanacorp	Cloranfenicol	41/AKD23	1
Sanacorp	Cloranfenicol	41/AKD24	1
Sannacorp	Cloranfenicol	2201014	1
Spangro 12.05.2014	Cloranfenicol	1308017-01	1
Spangro 14.03.2014	Cloranfenicol	12248524	1
Spangro_22.11.2018	Cloranfenicol	17343803	1
vdl	Cloranfenicol	12248501	1
VDL	Cloranfenicol	1308017-01	1
VDL	Cloranfenicol	140743-01	1

- 232 774 spectra from 1515 *Apo-Ident* customers from a total of 48 919 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloranfenicol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloranfenicol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	685	0	152 277
Type B	0	610	0	201 474
Type C	0	3288	5	232 774

The substance/substance group *Cloranfenicol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1241 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0164 %)
Type C	100.0000 % (> 99.9007 %)	99.8482 % (> 99.7571 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20777	20777	0,00	178,13
20787	20777	7,27	179,45
20807	20777	4,69	179,09
20813	20777	3,67	178,60
20815	20777	3,66	178,66
20822	20777	3,68	178,41
21701	21701	0,00	184,38
21752	22367	13,27	188,65

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21910	22367	3,26	183,89
21988	20777	7,23	181,39
22367	22367	0,00	181,91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloreto de alumínio hexa-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20131-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloreto de alumínio hexa-hidratado; Aluminii chloridum hexahydricum

Special notes

When selecting the *Cloreto de alumínio hexa-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloreto de alumínio hexa-hidratado	6	3	130

Second-stage model

For differentiation of the substance/substance group *Cloreto de alumínio hexa-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloreto de alumínio hexa-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	102,91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloreto de alumínio hexa-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloreto de alumínio hexa-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloreto de alumínio hexa-…	22002438	26556	40	20221121*
Euro OTC	Cloreto de alumínio hexa-…	1911008-03	26049	40	20210630
Euro OTC	Cloreto de alumínio hexa-…	2207005	26203	40	20220726*
Euro OTC	Cloreto de alumínio hexa-…	2207005	26203SI	20	20220726*
Fagron	Cloreto de alumínio hexa-…	21F07-B18-213240	26059	40	20211105
Fagron	Cloreto de alumínio hexa-…	23F22-B08-232244	27019	40	20230705
Fagron	Cloreto de alumínio hexa-…	23K16-B03-234491	27059	40	20231130

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Cloreto de alumínio hexa-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 6 reference samples from the substance/substance group *Cloreto de alumínio hexa-hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloreto de alumínio hexa-...	21002588	26053	40
Fagron	Cloreto de alumínio hexa-...	12I27-N01	20903	40
Fagron	Cloreto de alumínio hexa-...	23C23-B17-227778	26670	40
Caelo	Cloreto de alumínio hexa-...	21002588	26053SI	10
Euro OTC	Cloreto de alumínio hexa-...	1911008-03	26049SI†	10
Fagron	Cloreto de alumínio hexa-...	21F07-B18-213240	26059SI†	10

- 201 934 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 534 spectra from 240 *Apo-Ident* customers from 138 batches from the substance/substance group *Cloreto de alumínio hexa-hidratado*.

- Among them are spectra of independent samples from 130 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloreto de alumínio hexa-...	1911008-03	2
	Cloreto de alumínio hexa-...	1911008-04	3
	Cloreto de alumínio hexa-...	21002588002	1
	Cloreto de alumínio hexa-...	21002588006	1
	Cloreto de alumínio hexa-...	22002438001	9
	Cloreto de alumínio hexa-...	22002438002	5
	Cloreto de alumínio hexa-...	22002438003	1
	Cloreto de alumínio hexa-...	22002438005	3
	Cloreto de alumínio hexa-...	22002438006	6
	Cloreto de alumínio hexa-...	22002438008	2
	Cloreto de alumínio hexa-...	22002438010	7
	Cloreto de alumínio hexa-...	22002438012	1
	Cloreto de alumínio hexa-...	22002438013	1
	Cloreto de alumínio hexa-...	220700501	1
	Cloreto de alumínio hexa-...	2207005-01	18
	Cloreto de alumínio hexa-...	2207005-02	4
	Cloreto de alumínio hexa-...	22G29-B04	1
	Cloreto de alumínio hexa-...	22K14-B01-225235	1
	Cloreto de alumínio hexa-...	23c23-b17-227777	1
	Cloreto de alumínio hexa-...	23C23-B17-227777	3
	Cloreto de alumínio hexa-...	23k16-b03-234491	1
	Cloreto de alumínio hexa-...	7784-13-6	1
	Cloreto de alumínio hexa-...	K140A	1
5,56	Cloreto de alumínio hexa-...	22002438010	1
AHD	Cloreto de alumínio hexa-...	22002438001	1
AHD	Cloreto de alumínio hexa-...	22002438002	1
AHD	Cloreto de alumínio hexa-...	22002438012	1
AHD	Cloreto de alumínio hexa-...	22K14-B01-225218	2
Alliance Healthcare	Cloreto de alumínio hexa-...	13D22-N09	1
Alliance	Cloreto de alumínio hexa-...	21F07-B18-213240	1
Anzag	Cloreto de alumínio hexa-...	1204026-02	1
Caelo	Cloreto de alumínio hexa-...		2
Caelo	Cloreto de alumínio hexa-...	10251307	1
Caelo	Cloreto de alumínio hexa-...	10251314	1
Caelo	Cloreto de alumínio hexa-...	11229905	1
Caelo	Cloreto de alumínio hexa-...	11229906	1
Caelo	Cloreto de alumínio hexa-...	11229907	1
Caelo	Cloreto de alumínio hexa-...	11229914	1
Caelo	Cloreto de alumínio hexa-...	11229917	2
Caelo	Cloreto de alumínio hexa-...	12021303	1
Caelo	Cloreto de alumínio hexa-...	120402601	1
Caelo	Cloreto de alumínio hexa-...	1204026-01	3
Caelo	Cloreto de alumínio hexa-...	1204026-02	2
Caelo	Cloreto de alumínio hexa-...	12047503	2
Caelo	Cloreto de alumínio hexa-...	12047508	3
Caelo	Cloreto de alumínio hexa-...	12047512	1
Caelo	Cloreto de alumínio hexa-...	12047514	3
Caelo	Cloreto de alumínio hexa-...	1210014-01	3
Caelo	Cloreto de alumínio hexa-...	12114902	2
Caelo	Cloreto de alumínio hexa-...	12114904	2
Caelo	Cloreto de alumínio hexa-...	12114906	4
Caelo	Cloreto de alumínio hexa-...	12114908	7
Caelo	Cloreto de alumínio hexa-...	12114910	4
Caelo	Cloreto de alumínio hexa-...	12114912	4
Caelo	Cloreto de alumínio hexa-...	12114918	11
Caelo	Cloreto de alumínio hexa-...	12114919	1
Caelo	Cloreto de alumínio hexa-...	12114920	10
Caelo	Cloreto de alumínio hexa-...	12114922	13
Caelo	Cloreto de alumínio hexa-...	12323702	10
Caelo	Cloreto de alumínio hexa-...	12323710	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloreto de alumínio hexa-...	12323711	12
Caelo	Cloreto de alumínio hexa-...	12323717	4
Caelo	Cloreto de alumínio hexa-...	12C07-N01	2
Caelo	Cloreto de alumínio hexa-...	12i27-N01	1
Caelo	Cloreto de alumínio hexa-...	12I27-N01	1
Caelo	Cloreto de alumínio hexa-...	12l27-N01	2
Caelo	Cloreto de alumínio hexa-...	12l27-N01	1
Caelo	Cloreto de alumínio hexa-...	13/13-B03-287298	1
Caelo	Cloreto de alumínio hexa-...	13D22-N09	3
Caelo	Cloreto de alumínio hexa-...	13G03-N02	2
Caelo	Cloreto de alumínio hexa-...	13L13-B03-287298	1
Caelo	Cloreto de alumínio hexa-...	15051302	1
Caelo	Cloreto de alumínio hexa-...	15080701	1
Caelo	Cloreto de alumínio hexa-...	15080715	1
Caelo	Cloreto de alumínio hexa-...	18061308	1
Caelo	Cloreto de alumínio hexa-...	18261314	1
Caelo	Cloreto de alumínio hexa-...	19041302	1
Caelo	Cloreto de alumínio hexa-...	23111203	1
Caelo	Cloreto de alumínio hexa-...	28121301	1
Caelo	Cloreto de alumínio hexa-...	3091205	1
Caelo	Cloreto de alumínio hexa-...	3113E-01095	1
Caelo	Cloreto de alumínio hexa-...	5081301	1
Caelo	Cloreto de alumínio hexa-...	51/AD1	1
Caelo	Cloreto de alumínio hexa-...	8031301	1
Caelo	Cloreto de alumínio hexa-...	9071303	1
Caelo	Cloreto de alumínio hexa-...	C181A	1
Caesar & Loretz GmbH...	Cloreto de alumínio hexa-...	12114918	4
Caesar & Loretz GmbH...	Cloreto de alumínio hexa-...	12047508	1
Caesar & Loretz GmbH...	Cloreto de alumínio hexa-...	12114906	1
Caesar & Loretz GmbH...	Cloreto de alumínio hexa-...	12323702	1
Caesar & Loretz GmbH...	Cloreto de alumínio hexa-...	12323711	2
Caesar & Loretz GmbH	Cloreto de alumínio hexa-...	12114906	1
Caesar & Loretz GmbH	Cloreto de alumínio hexa-...	12114918	1
Caesar & Loretz GmbH	Cloreto de alumínio hexa-...	12323702	1
Caesar/Lorenz	Cloreto de alumínio hexa-...	12114918	1
Eurho / Sanacorp	Cloreto de alumínio hexa-...	12I27-N01	1
EuRho Pharm	Cloreto de alumínio hexa-...	1109025-02	1
EuRho	Cloreto de alumínio hexa-...	1106017-01	1
EuRho	Cloreto de alumínio hexa-...	1210014-01	1
EuRho	Cloreto de alumínio hexa-...	2512I01095	1
EuRho	Cloreto de alumínio hexa-...	d024a	1
Euro OTC	Cloreto de alumínio hexa-...	1103007-01	1
Euro OTC	Cloreto de alumínio hexa-...	1109025-01	1
Euro OTC	Cloreto de alumínio hexa-...	1109025-02	1
Euro OTC	Cloreto de alumínio hexa-...	120402601	1
Euro OTC	Cloreto de alumínio hexa-...	1204026-01	16
Euro OTC	Cloreto de alumínio hexa-...	120402602	1
Euro OTC	Cloreto de alumínio hexa-...	1204026-02	13
Euro OTC	Cloreto de alumínio hexa-...	12100014-02	1
Euro OTC	Cloreto de alumínio hexa-...	1210012-01	1
Euro OTC	Cloreto de alumínio hexa-...	121001401	2
Euro OTC	Cloreto de alumínio hexa-...	1210014-01	18
Euro OTC	Cloreto de alumínio hexa-...	121001402	1
Euro OTC	Cloreto de alumínio hexa-...	1210014-02	24
Euro OTC	Cloreto de alumínio hexa-...	1210014-02-336331909	1
Euro OTC	Cloreto de alumínio hexa-...	1213M-01095	1
Euro OTC	Cloreto de alumínio hexa-...	1307011	1
Euro OTC	Cloreto de alumínio hexa-...	1307011-01	10
Euro OTC	Cloreto de alumínio hexa-...	1307011-02	2
Euro OTC	Cloreto de alumínio hexa-...	1406021-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloreto de alumínio hexa-…	1507002-01	1
Euro OTC	Cloreto de alumínio hexa-…	2111Q-01095	1
Euro OTC	Cloreto de alumínio hexa-…	2207005-01	1
Euro OTC	Cloreto de alumínio hexa-…	co31a	1
EUro/AHD	Cloreto de alumínio hexa-…	121001401	1
EUro/AHD	Cloreto de alumínio hexa-…	1210014-01	1
Euroo/Phoenix	Cloreto de alumínio hexa-…	120014-02	1
Euroo/Phoenix	Cloreto de alumínio hexa-…	1210014-02	2
Fagron	Cloreto de alumínio hexa-…		1
Fagron	Cloreto de alumínio hexa-…	105282-0001	1
Fagron	Cloreto de alumínio hexa-…	11/23-N06	1
Fagron	Cloreto de alumínio hexa-…	11/23-N06B206A	1
Fagron	Cloreto de alumínio hexa-…	11G05-N02	1
Fagron	Cloreto de alumínio hexa-…	11G05-No2	1
Fagron	Cloreto de alumínio hexa-…	11l23-N06	3
Fagron	Cloreto de alumínio hexa-…	12/11-No3	1
Fagron	Cloreto de alumínio hexa-…	12/27/N01	1
Fagron	Cloreto de alumínio hexa-…	12/27-n01	1
Fagron	Cloreto de alumínio hexa-…	12/27-N01	5
Fagron	Cloreto de alumínio hexa-…	12047512	1
Fagron	Cloreto de alumínio hexa-…	1207211095	1
Fagron	Cloreto de alumínio hexa-…	12082013D	1
Fagron	Cloreto de alumínio hexa-…	12323702	2
Fagron	Cloreto de alumínio hexa-…	12323711	1
Fagron	Cloreto de alumínio hexa-…	12C07-N01	4
Fagron	Cloreto de alumínio hexa-…	12G05-N10	23
Fagron	Cloreto de alumínio hexa-…	12i27-N01	1
Fagron	Cloreto de alumínio hexa-…	12I27-N01	9
Fagron	Cloreto de alumínio hexa-…	12L11-N03	2
Fagron	Cloreto de alumínio hexa-…	12l27-N01	2
Fagron	Cloreto de alumínio hexa-…	13126-N13	1
Fagron	Cloreto de alumínio hexa-…	13D22N09	2
Fagron	Cloreto de alumínio hexa-…	13D22-N09	19
Fagron	Cloreto de alumínio hexa-…	13d22no9	1
Fagron	Cloreto de alumínio hexa-…	13G03-N02	19
Fagron	Cloreto de alumínio hexa-…	13I26-N13	2
Fagron	Cloreto de alumínio hexa-…	13J31-B06-287615	1
Fagron	Cloreto de alumínio hexa-…	17F26-B01-340253	1
Fagron	Cloreto de alumínio hexa-…	1910211095	1
Fagron	Cloreto de alumínio hexa-…	20122013E	1
Fagron	Cloreto de alumínio hexa-…	2013U-01095	1
Fagron	Cloreto de alumínio hexa-…	2913U1095	1
Fagron	Cloreto de alumínio hexa-…	5213A1095	1
Fagron	Cloreto de alumínio hexa-…	8547287	1
Fagron	Cloreto de alumínio hexa-…	C012A	1
Fagron	Cloreto de alumínio hexa-…	C145A	1
Fagron	Cloreto de alumínio hexa-…	C181A	1
Fargon	Cloreto de alumínio hexa-…	11/23-N06	1
Faron	Cloreto de alumínio hexa-…	13I13-B03-287298	1
Fragon	Cloreto de alumínio hexa-…	13D22-N09	1
Gehe	Cloreto de alumínio hexa-…	11229917	1
Gehe	Cloreto de alumínio hexa-…	120402601	1
Gehe	Cloreto de alumínio hexa-…	12047512	1
Gehe	Cloreto de alumínio hexa-…	1210014-01	2
Gehe	Cloreto de alumínio hexa-…	12114902	1
Gehe	Cloreto de alumínio hexa-…	12114908	1
Gehe	Cloreto de alumínio hexa-…	12114922	1
Gehe	Cloreto de alumínio hexa-…	12323711	2
Gehe	Cloreto de alumínio hexa-…	130701102	1
Gehe	Cloreto de alumínio hexa-…	1911008-04	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Cloreto de alumínio hexa-…	21002588009	1
Gehe	Cloreto de alumínio hexa-…	22002438001	1
Gehe	Cloreto de alumínio hexa-…	22002438005	1
Gehe	Cloreto de alumínio hexa-…	2207005-01	1
Gehe	Cloreto de alumínio hexa-…	23C23-B17-227777	1
Honeywell	Cloreto de alumínio hexa-…	1210014-02	1
Ichthyol-Gesellschaf…	Cloreto de alumínio hexa-…	12114918	1
Krömpke	Cloreto de alumínio hexa-…	1204026-01	1
Noweda	Cloreto de alumínio hexa-…	1109025-02	1
Noweda	Cloreto de alumínio hexa-…	12114910	2
Noweda	Cloreto de alumínio hexa-…	191008-04	1
Noweda	Cloreto de alumínio hexa-…	21K26-B04-216815	1
Noweda	Cloreto de alumínio hexa-…	22002438001	2
Noweda	Cloreto de alumínio hexa-…	22002438006	1
NOWEDA	Cloreto de alumínio hexa-…	22002438006	1
Noweda	Cloreto de alumínio hexa-…	2207005-01	3
Noweda	Cloreto de alumínio hexa-…	22K14-B01-225219	1
Phoenix	Cloreto de alumínio hexa-…	1210014-01	1
Phoenix	Cloreto de alumínio hexa-…	13D22-N09	1
Phoenix	Cloreto de alumínio hexa-…	2207005-01	1
Phönix Gotha	Cloreto de alumínio hexa-…	1210014-02	1
Phönix	Cloreto de alumínio hexa-…	12/27-N01	1
Phönix	Cloreto de alumínio hexa-…	1204026-02	1
Phönix	Cloreto de alumínio hexa-…	1210014-02	1
Phönix	Cloreto de alumínio hexa-…	12L11-N03	1
Phönix	Cloreto de alumínio hexa-…	22002438001	1
Phönix	Cloreto de alumínio hexa-…	22002438010	1
Phönix	Cloreto de alumínio hexa-…	2207005-01	1
Sanacorp	Cloreto de alumínio hexa-…	1210014-02	1
Sanacorp	Cloreto de alumínio hexa-…	12114920	1
Sanacorp	Cloreto de alumínio hexa-…	12323717	1
Sanacorp	Cloreto de alumínio hexa-…	12C07-N01	1
Sanacorp	Cloreto de alumínio hexa-…	22002438001	1
Sanacorp	Cloreto de alumínio hexa-…	22002438010	1
Sanacorp	Cloreto de alumínio hexa-…	2207005-01	2
Sanacorp	Cloreto de alumínio hexa-…	22G29-B04-220832	1
vdL	Cloreto de alumínio hexa-…	2207005-01	1

- 235 533 spectra from 1515 *Apo-Ident* customers from a total of 49 122 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloreto de alumínio hexa-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloreto de alumínio hexa-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	150	0	201 934
Type C	0	530	4	235 533

The substance/substance group *Cloreto de alumínio hexa-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.2509 % (> 98.6891 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26049	26556	14,27	174,75
26059	26556	11,52	182,18
26203	26203	0,00	175,06
26556	26556	0,00	183,76
27019	26203	7,52	179,46
27059	26203	11,19	184,35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloreto de colina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22639-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloreto de colina; Cholinii chloridum; Colina, cloreto

Special notes

When selecting the *Cloreto de colina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloreto de colina	6	4	0

Second-stage model

For differentiation of the substance/substance group *Cloreto de colina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloreto de colina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	111,37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloreto de colina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloreto de colina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloreto de colina	162092	22639	40	20160801*
Caelo	Cloreto de colina	14273819	22663	40	20141002
Caelo	Cloreto de colina	14273819	22734	40	20141002
Caelo	Cloreto de colina	16209209	23582	40	20160801
Caelo	Cloreto de colina	20001839	25557	40	20200721*
Caelo	Cloreto de colina	21002730	25853	50	20210908*
Fagron	Cloreto de colina	23C20-B09-230712	26918	40	20230424
Fagron	Cloreto de colina	23C20-B09-230712	26918SI	20	20230424

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 310 spectra of 8 reference samples from the substance/substance group *Cloreto de colina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 652 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Cloreto de colina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloreto de colina	172053	23618	40
Caelo	Cloreto de colina	181082	24264	40
Caelo	Cloreto de colina	20003488	25662	40
Caelo	Cloreto de colina	22000199	25990	40
Caelo	Cloreto de colina	22000199	25990SI	10

- 201 914 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloreto de colina*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloreto de colina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloreto de colina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	170	0	201 914
Type C	0	0	0	236 067

The substance/substance group *Cloreto de colina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22639	22639	0,00	141,53
22663	25853	18,04	140,21
22734	25853	17,41	139,47
23582	22639	10,91	139,43
25557	25557	0,00	151,01
25853	25853	0,00	142,78
26918	25853	10,75	141,34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloreto de dequalínio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20350-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloreto de dequalínio; Dequalinii chloridum

Special notes

When selecting the *Cloreto de dequalínio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloreto de dequalínio	13	7	129

Second-stage model

For differentiation of the substance/substance group *Cloreto de dequalínio* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloreto de dequalínio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	72,04	–
⋮	⋮	⋮
Ditranol	>50	59,83
Eosina amarela	>50	96,32
Cloridrato de oxitetraciclina	>50	133,02
Salicilato de sódio	>50	143,24
Levotiroxina sódica	>50	184,62
Tanino	>50	252,26
Ácido acetilsalicílico	>50	255,42
Ácido benzoico	>50	433,75

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloreto de dequalínio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloreto de dequalínio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloreto de dequalínio	12361908	21296	40	1412076
Caelo	Cloreto de dequalínio	12361906	21387	60	20121228
Caelo	Cloreto de dequalínio	15218406	22953	40	20150622
Caelo	Cloreto de dequalínio	15402803	23121	40	1707614
Caelo	Cloreto de dequalínio	154028	23362	40	20160219*
Caelo	Cloreto de dequalínio	154028	24403	40	20160219*
Caelo	Cloreto de dequalínio	191314	25205	40	20190626*
Euro OTC	Cloreto de dequalínio	1405012-01	21617	60	20140623
Euro OTC	Cloreto de dequalínio	1512032	22295	60	20160121*
Euro OTC	Cloreto de dequalínio	1512032-02	24142	40	1809202
Euro OTC	Cloreto de dequalínio	2003008	25156	40	20200528*
Euro OTC	Cloreto de dequalínio	2103018	25687	40	20210421*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloreto de dequalínio	13I26-N10	21269	40	20130121
Fagron	Cloreto de dequalínio	15B16-B04-332113	23266	40	20150226

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 620 spectra of 14 reference samples from the substance/substance group *Cloreto de dequalínio*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 342 spectra from a total of 2829 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 500 spectra of 12 reference samples from the substance/substance group *Cloreto de dequalínio*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloreto de dequalínio	180794	24011	40
Caelo	Cloreto de dequalínio	22001564	26243	40
Caelo	Cloreto de dequalínio	24001318	27314	40
Euro OTC	Cloreto de dequalínio	1804009	24082	40
Euro OTC	Cloreto de dequalínio	2310016	27194	40
Fagron	Cloreto de dequalínio	11D29-N11	20660	80
Fagron	Cloreto de dequalínio	19J16-B08-197304	25177	40
Caelo	Cloreto de dequalínio	12361906	21386	60
Caelo	Cloreto de dequalínio	12361906	21387†	60
Caelo	Cloreto de dequalínio	22001564	26243SI	20
Caelo	Cloreto de dequalínio	24001318	27314SI	20
Euro OTC	Cloreto de dequalínio	2310016	27194SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 584 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 498 spectra from 309 *Apo-Ident* customers from 138 batches from the substance/substance group *Cloreto de dequalínio*.
- Among them are spectra of independent samples from 124 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloreto de dequalínio	20003344009	1
	Cloreto de dequalínio	20003344010	2
	Cloreto de dequalínio	2103018-01	3
	Cloreto de dequalínio	22001564003	2
	Cloreto de dequalínio	22001564004	2
	Cloreto de dequalínio	22001564008	1
	Cloreto de dequalínio	22001564013	1
AHD	Cloreto de dequalínio	15218401	1
Alliance H.	Cloreto de dequalínio	1512032-01	1
Alliance Health	Cloreto de dequalínio	12077508	1
Alliance Healthcare	Cloreto de dequalínio	19131402	1
Alliance Healthcare	Cloreto de dequalínio	2003008-01	1
Allianz Healthcare	Cloreto de dequalínio	1512032-01	1
Anzag ek:7.89EUR	Cloreto de dequalínio	11166204	1
Anzag	Cloreto de dequalínio	15B16-B04-340177	1
apomix	Cloreto de dequalínio	1804009-01	1
Caelo	Cloreto de dequalínio		1
Caelo	Cloreto de dequalínio	10879409	1
Caelo	Cloreto de dequalínio	11166203	1
Caelo	Cloreto de dequalínio	11166204	2
Caelo	Cloreto de dequalínio	11166209	1
Caelo	Cloreto de dequalínio	12077508	2
Caelo	Cloreto de dequalínio	12077510	7
Caelo	Cloreto de dequalínio	1210008-03	1
Caelo	Cloreto de dequalínio	12361906	3
Caelo	Cloreto de dequalínio	12361908	2
Caelo	Cloreto de dequalínio	12361911	3
Caelo	Cloreto de dequalínio	12G05-N07	1
Caelo	Cloreto de dequalínio	13/26-N10	1
Caelo	Cloreto de dequalínio	13348805	2
Caelo	Cloreto de dequalínio	13A23-N02	2
Caelo	Cloreto de dequalínio	1405012-02	1
Caelo	Cloreto de dequalínio	14072901	1
Caelo	Cloreto de dequalínio	14C10-B03	1
Caelo	Cloreto de dequalínio	151203202	1
Caelo	Cloreto de dequalínio	1512032-02	3
Caelo	Cloreto de dequalínio	152184	1
Caelo	Cloreto de dequalínio	15218401	7

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloreto de dequalínio	15218402	1
Caelo	Cloreto de dequalínio	15218404	2
Caelo	Cloreto de dequalínio	15218406	6
Caelo	Cloreto de dequalínio	15218407	1
Caelo	Cloreto de dequalínio	15218410	1
Caelo	Cloreto de dequalínio	15402801	3
Caelo	Cloreto de dequalínio	15402803	4
Caelo	Cloreto de dequalínio	15402805	2
Caelo	Cloreto de dequalínio	15402806	2
Caelo	Cloreto de dequalínio	15402807	2
Caelo	Cloreto de dequalínio	15B16-B04	1
Caelo	Cloreto de dequalínio	15B16-B04-326872	1
Caelo	Cloreto de dequalínio	15B16-B04-337594	1
Caelo	Cloreto de dequalínio	15B16-B04-342302	1
Caelo	Cloreto de dequalínio	18015801	2
Caelo	Cloreto de dequalínio	18015802	2
Caelo	Cloreto de dequalínio	1804009-03	2
Caelo	Cloreto de dequalínio	18079402	1
Caelo	Cloreto de dequalínio	18079403	6
Caelo	Cloreto de dequalínio	18079404	3
Caelo	Cloreto de dequalínio	18079405	1
Caelo	Cloreto de dequalínio	18079407	3
Caelo	Cloreto de dequalínio	18079408	1
Caelo	Cloreto de dequalínio	18079410	1
Caelo	Cloreto de dequalínio	18079411	3
Caelo	Cloreto de dequalínio	191314003	8
Caelo	Cloreto de dequalínio	191314004	6
Caelo	Cloreto de dequalínio	191314005	1
Caelo	Cloreto de dequalínio	191314006	2
Caelo	Cloreto de dequalínio	19131402	10
Caelo	Cloreto de dequalínio	20003344004	6
Caelo	Cloreto de dequalínio	20003344006	1
Caelo	Cloreto de dequalínio	20003344007	2
Caelo	Cloreto de dequalínio	20003344009	2
Caelo	Cloreto de dequalínio	20003344012	3
Caelo	Cloreto de dequalínio	2000334404	1
Caelo	Cloreto de dequalínio	2003008-01	2
Caelo	Cloreto de dequalínio	215I-01325	1
Caelo	Cloreto de dequalínio	22001564002	1
Caelo	Cloreto de dequalínio	220812K2	1
Caelo	Cloreto de dequalínio	3613A-01325	1
Caelo	Cloreto de dequalínio	5315I-01325	1
Caeol/Noweda	Cloreto de dequalínio	19131402	2
Caesar & Loretz GmbH...	Cloreto de dequalínio	18079411	1
Caesar & Loretz GmbH...	Cloreto de dequalínio	191314007	1
Caesar & Loretz GmbH...	Cloreto de dequalínio	20003344003	1
Caesar & Loretz GmbH...	Cloreto de dequalínio	20003344007	1
Caesar & Loretz GmbH	Cloreto de dequalínio	18079404	2
Caesar & Loretz GmbH	Cloreto de dequalínio	18079410	1
Caesar & Loretz GmbH	Cloreto de dequalínio	18079411	1
Caesar & Loretz GmbH	Cloreto de dequalínio	191314003	3
Caesar & Loretz GmbH	Cloreto de dequalínio	191314004	1
Caesar & Loretz GmbH	Cloreto de dequalínio	191314006	2
Caesar & Loretz GmbH	Cloreto de dequalínio	191314007	3
Caesar & Loretz GmbH	Cloreto de dequalínio	19131402	5
Caesar & Loretz GmbH	Cloreto de dequalínio	20003344004	2
Caesar & Loretz GmbH	Cloreto de dequalínio	210008690091	1
Caesar & Loretz GmbH	Cloreto de dequalínio	22001564002	1
Cealo, GEHE	Cloreto de dequalínio	2003008-01	1
Eurho Sanacorp	Cloreto de dequalínio	2003008-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/ Anzag	Cloreto de dequalínio	220627(2103018-01)	1
EuRho/ Anzag	Cloreto de dequalínio	80(1804009-01)	1
EuRho/Gehe	Cloreto de dequalínio	2003008-01	2
EuRho/Phoenix	Cloreto de dequalínio	2103018-01	1
EuRho	Cloreto de dequalínio	1110002-01	1
EuRho	Cloreto de dequalínio	2003008-01	1
Euro OTC	Cloreto de dequalínio		3
Euro OTC	Cloreto de dequalínio	1010022-01	2
Euro OTC	Cloreto de dequalínio	1103045-01	1
Euro OTC	Cloreto de dequalínio	11091701	1
Euro OTC	Cloreto de dequalínio	1110002-01	2
Euro OTC	Cloreto de dequalínio	1210008-01	2
Euro OTC	Cloreto de dequalínio	1210008-02	2
Euro OTC	Cloreto de dequalínio	1210008-03	2
Euro OTC	Cloreto de dequalínio	1405012-01	5
Euro OTC	Cloreto de dequalínio	1405012-02	6
Euro OTC	Cloreto de dequalínio	1407029-01	7
Euro OTC	Cloreto de dequalínio	1407029-02	6
Euro OTC	Cloreto de dequalínio	15061204	1
Euro OTC	Cloreto de dequalínio	151203201	1
Euro OTC	Cloreto de dequalínio	1512032-01	21
Euro OTC	Cloreto de dequalínio	1512032-02	13
Euro OTC	Cloreto de dequalínio	180400901	1
Euro OTC	Cloreto de dequalínio	1804009-01	20
Euro OTC	Cloreto de dequalínio	1804009-02	4
Euro OTC	Cloreto de dequalínio	1804009-03	22
Euro OTC	Cloreto de dequalínio	18040092-02	1
Euro OTC	Cloreto de dequalínio	18044009-01	1
Euro OTC	Cloreto de dequalínio	2000300801	1
Euro OTC	Cloreto de dequalínio	20030008-01	1
Euro OTC	Cloreto de dequalínio	2003008-01	23
Euro OTC	Cloreto de dequalínio	2103018-01	20
Euro OTC	Cloreto de dequalínio	210318-01	1
Euro OTC	Cloreto de dequalínio	211118(2003008)	1
Euro OTC	Cloreto de dequalínio	220809(2103018-01)	1
Euro OTC	Cloreto de dequalínio	804009-021	1
Euro OTC	Cloreto de dequalínio	81(1804009-01)	1
Euro OTC	Cloreto de dequalínio	EuroOTC	1
Euro/Sanacorp	Cloreto de dequalínio	1512032-02	1
Euro/Spangro	Cloreto de dequalínio	1512032-02	1
Fag / Noweda	Cloreto de dequalínio	15B16-B04-321326	1
Fagron	Cloreto de dequalínio		5
Fagron	Cloreto de dequalínio	10H05-N07	1
Fagron	Cloreto de dequalínio	12B14-N01	1
Fagron	Cloreto de dequalínio	12D05-N09	1
Fagron	Cloreto de dequalínio	12G05-N07	2
Fagron	Cloreto de dequalínio	13A23-N02	3
Fagron	Cloreto de dequalínio	13D26-N06	3
Fagron	Cloreto de dequalínio	13I26-N10	1
Fagron	Cloreto de dequalínio	1407029-01	2
Fagron	Cloreto de dequalínio	14C10-B03	1
Fagron	Cloreto de dequalínio	14C10B03292286	1
Fagron	Cloreto de dequalínio	14C10-B03-292286	4
Fagron	Cloreto de dequalínio	15B16-B04	2
Fagron	Cloreto de dequalínio	15B16B04304432	1
Fagron	Cloreto de dequalínio	15B16-B04-304432	2
Fagron	Cloreto de dequalínio	15B16-B04-316267	4
Fagron	Cloreto de dequalínio	15B16B04321326	1
Fagron	Cloreto de dequalínio	15B16-B04-321326	1
Fagron	Cloreto de dequalínio	15B16-B04-326872	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloreto de dequalínio	15B16-B04-332113	3
Fagron	Cloreto de dequalínio	15B16B04337594	1
Fagron	Cloreto de dequalínio	15B16-B04-340177	1
Fagron	Cloreto de dequalínio	15B16-B04-342302	2
Fagron	Cloreto de dequalínio	15B16-B04-346969	4
Fagron	Cloreto de dequalínio	15B16-B04-352989	2
Fagron	Cloreto de dequalínio	15B16-B04-354618	2
Fagron	Cloreto de dequalínio	18B16-B04-356149	1
Fagron	Cloreto de dequalínio	19J16-B08	4
Fagron	Cloreto de dequalínio	19J16B08197304	2
Fagron	Cloreto de dequalínio	19J16-B08-197304	8
Fagron	Cloreto de dequalínio	19JI-B08-197304	1
Fagron	Cloreto de dequalínio	20F19-B03-201436	6
Fagron	Cloreto de dequalínio	20I18-B01-202442	2
Fagron	Cloreto de dequalínio	B03_2014306	1
Fagron	Cloreto de dequalínio	B03-2014306	3
Fiebig	Cloreto de dequalínio	2003008-01	1
Gatt-Koller	Cloreto de dequalínio	1800212	1
GEHE/ EuRho	Cloreto de dequalínio	2103018-01	1
Gehe/EuRho	Cloreto de dequalínio	9245-90125	1
Gehe	Cloreto de dequalínio	1512032-01	1
GEHE	Cloreto de dequalínio	1804009-01	1
GUMO	Cloreto de dequalínio	191314003	1
Klosterring	Cloreto de dequalínio	15B16-B04-321326	1
L30	Cloreto de dequalínio	1804009-01	1
Lamotte/Spangroh	Cloreto de dequalínio	15218404	1
Lebsa/AHD	Cloreto de dequalínio	1405012-01	1
LEBSA/Phoenix	Cloreto de dequalínio	1210008-03	1
LEBSA	Cloreto de dequalínio		1
Lebsa	Cloreto de dequalínio	2003008-01	2
Nachprüfung	Cloreto de dequalínio	2082019-10	1
Noweda	Cloreto de dequalínio	12b14-n05	1
Ph.Euro/Noweda	Cloreto de dequalínio	2103018-01	1
Phoenix	Cloreto de dequalínio	191314006	1
Phönix/EuRo	Cloreto de dequalínio	2003008-01	1
Phönix/Fagon	Cloreto de dequalínio	15B16-B04-316267	1
Phönix	Cloreto de dequalínio	10127-N02Retest	1
Phönix	Cloreto de dequalínio	1110002-01	1
Phönix	Cloreto de dequalínio	13D26-N06	1
Phönix	Cloreto de dequalínio	151203201	1
Phönix	Cloreto de dequalínio	1804009-01	1
phönix	Cloreto de dequalínio	2103018-01	1
Raben-Apotheke Mildenau	Cloreto de dequalínio	1405012-01	1
S.Binder	Cloreto de dequalínio	1210008-04	1
Sanacorp	Cloreto de dequalínio	18079407	2
Sanacorp	Cloreto de dequalínio	19131402	1
Th. Geyer	Cloreto de dequalínio	15B16-B04-354618	1
Wepa Apothekenbedarf	Cloreto de dequalínio	151203202	1

- 235 569 spectra from 1515 *Apo-Ident* customers from a total of 49 121 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloreto de dequalínio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

all relevant spectra of the various substances were compared with *Cloreto de dequalínio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	500	0	201 584
Type C	0	497	1	235 569

The substance/substance group *Cloreto de dequalínio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.9007 %)	99.7992 % (> 99.1968 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21269	21296	50,39	149,16
21296	21296	0,00	170,94
21387	21296	13,94	174,93
21617	21296	28,41	190,82
22295	22295	0,00	203,31
22953	21296	38,21	152,53
23121	23121	0,00	268,13
23266	23362	38,27	233,54
23362	23362	0,00	213,82
24142	24142	0,00	144,92
24403	24403	0,00	163,84
25156	25156	0,00	258,31
25205	25205	0,00	152,61
25687	25687	0,00	246,45

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloreto de magnésio hexa-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006390-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloreto de magnésio hexa-hidratado; Magnesii chloridum hexahydricum

Special notes

When selecting the *Cloreto de magnésio hexa-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloreto de magnésio hexa-hidratado	3	1	68

Second-stage model

For differentiation of the substance/substance group *Cloreto de magnésio hexa-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloreto de magnésio hexa-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	86,19	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloreto de magnésio hexa-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloreto de magnésio hexa-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloreto de magnésio hexa-...	1802023-01	24275	40	20180223
Euro OTC	Cloreto de magnésio hexa-...	2107014	25790	50	20210812*
Euro OTC	Cloreto de magnésio hexa-...	2307025	27085	40	20230810*
Euro OTC	Cloreto de magnésio hexa-...	2307025	27085SI	20	20230810*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 150 spectra of 4 reference samples from the substance/substance group *Cloreto de magnésio hexa-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 812 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Cloreto de magnésio hexa-hidratado*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloreto de magnésio hexa-…	24A22-B03-235953	27267	40
Fagron	Cloreto de magnésio hexa-…	24A22-B03-235953	27267SI	20

- 202 024 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 139 spectra from 49 *Apo-Ident* customers from 72 batches from the substance/substance group *Cloreto de magnésio hexa-hidratado*.

- Among them are spectra of independent samples from 67 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Anzag	Cloreto de magnésio hexa-…	120802501	1
Anzag	Cloreto de magnésio hexa-…	1304003-01	1
Caelo	Cloreto de magnésio hexa-…		1
Caelo	Cloreto de magnésio hexa-…	1108024-01	1
Caelo	Cloreto de magnésio hexa-…	11345606	1
Caelo	Cloreto de magnésio hexa-…	11345609	1
Caelo	Cloreto de magnésio hexa-…	11345623	2
Caelo	Cloreto de magnésio hexa-…	11345624	1
Caelo	Cloreto de magnésio hexa-…	12141803	1
Caelo	Cloreto de magnésio hexa-…	12141806	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloreto de magnésio hexa-…	12141807	3
Caelo	Cloreto de magnésio hexa-…	12141808	1
Caelo	Cloreto de magnésio hexa-…	12141811	2
Caelo	Cloreto de magnésio hexa-…	12141814	1
Caelo	Cloreto de magnésio hexa-…	12141817	2
Caelo	Cloreto de magnésio hexa-…	12354604	4
Caelo	Cloreto de magnésio hexa-…	12354605	4
Caelo	Cloreto de magnésio hexa-…	12354606	4
Caelo	Cloreto de magnésio hexa-…	12354608	1
Caelo	Cloreto de magnésio hexa-…	12354609	7
Caelo	Cloreto de magnésio hexa-…	12354610	2
Caelo	Cloreto de magnésio hexa-…	12354612	7
Caelo	Cloreto de magnésio hexa-…	12354613	4
Caelo	Cloreto de magnésio hexa-…	12354615	8
Caelo	Cloreto de magnésio hexa-…	12354618	2
Caelo	Cloreto de magnésio hexa-…	1304C004	1
Caelo	Cloreto de magnésio hexa-…	13194701	1
Caelo	Cloreto de magnésio hexa-…	13194702	3
Caelo	Cloreto de magnésio hexa-…	13194706	3
Caelo	Cloreto de magnésio hexa-…	13194707	4
Caelo	Cloreto de magnésio hexa-…	13194713	1
Caelo	Cloreto de magnésio hexa-…	13194713-3490312103	1
Caelo	Cloreto de magnésio hexa-…	13194721	2
Caelo	Cloreto de magnésio hexa-…	1512I-01828	1
Caelo	Cloreto de magnésio hexa-…	16094004	1
Caelo	Cloreto de magnésio hexa-…	16094014	1
Caelo	Cloreto de magnésio hexa-…	17034304	1
Caelo	Cloreto de magnésio hexa-…	5210I-01828	1
Caesar & Loretz GmbH	Cloreto de magnésio hexa-…	13064223	1
Cealo	Cloreto de magnésio hexa-…	112354615	1
Cealo	Cloreto de magnésio hexa-…	11354615	1
Euro OTC	Cloreto de magnésio hexa-…	1112013-01	2
Euro OTC	Cloreto de magnésio hexa-…	1204017-01	1
Euro OTC	Cloreto de magnésio hexa-…	1208025-01	1
Euro OTC	Cloreto de magnésio hexa-…	1212013-01	3
Euro OTC	Cloreto de magnésio hexa-…	1304003-01	1
Fagron	Cloreto de magnésio hexa-…	11K17-N10	1
Fagron	Cloreto de magnésio hexa-…	12B16-N01	1
Fagron	Cloreto de magnésio hexa-…	12D11-N01	1
Fagron	Cloreto de magnésio hexa-…	12h21-N02	1
Fagron	Cloreto de magnésio hexa-…	12H21-N02	5
Fagron	Cloreto de magnésio hexa-…	12H21-No2	1
Fagron	Cloreto de magnésio hexa-…	12H21-NO2	1
Fagron	Cloreto de magnésio hexa-…	1301c009-277802	1
Fagron	Cloreto de magnésio hexa-…	1301C009-277802	4
Fagron	Cloreto de magnésio hexa-…	1301C011-277803	1
Fagron	Cloreto de magnésio hexa-…	1301C012-277804	1
Fagron	Cloreto de magnésio hexa-…	1301C10	3
Fagron	Cloreto de magnésio hexa-…	1301C10-277801	1
Fagron	Cloreto de magnésio hexa-…	1304C001-281211	2
Fagron	Cloreto de magnésio hexa-…	1304C002	1
Fagron	Cloreto de magnésio hexa-…	1304C003	1
Fagron	Cloreto de magnésio hexa-…	1304C003-281209	1
Fagron	Cloreto de magnésio hexa-…	1304C004	1
Fagron	Cloreto de magnésio hexa-…	1304c004-281210	1
Fagron	Cloreto de magnésio hexa-…	1304C004-281210	1
Fagron	Cloreto de magnésio hexa-…	13411207	1
Fagron	Cloreto de magnésio hexa-…	13B14-B01-287292	1
Fagron	Cloreto de magnésio hexa-…	26061305	1
Fagron	Cloreto de magnésio hexa-…	M1430	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloreto de magnésio hexa-…	M1555	1
Fagron	Cloreto de magnésio hexa-…	M1625	1
Fragon/Sanacorp	Cloreto de magnésio hexa-…	12H21-N02	4
Phönix/Euro	Cloreto de magnésio hexa-…	1208025-01	1
stumpf	Cloreto de magnésio hexa-…	1301c012-277804	1
unbekannt	Cloreto de magnésio hexa-…	unbekannt	1

- 235 928 spectra from 1515 *Apo-Ident* customers from a total of 49 187 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloreto de magnésio hexa-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloreto de magnésio hexa-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	150	0	152 812
Type B	0	60	0	202 024
Type C	0	108	31	235 928

The substance/substance group *Cloreto de magnésio hexa-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9007 %)	77.6978 % (> 75.5396 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24275	27085	21,08	152,02
25790	25790	0,00	159,37
27085	27085	0,00	155,46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloreto de metacolina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20733-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloreto de metacolina; Methacholinii chloridum

Special notes

When selecting the *Cloreto de metacolina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloreto de metacolina	9	5	30

Second-stage model

For differentiation of the substance/substance group *Cloreto de metacolina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloreto de metacolina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aspartato de ornitina	118,89	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloreto de metacolina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloreto de metacolina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloreto de metacolina	13260303	21251	40	20130827
Caelo	Cloreto de metacolina	13260302	21420	60	20130827
Caelo	Cloreto de metacolina	13260302	21590	60	20130827
Caelo	Cloreto de metacolina	13260303	21592	60	20130827
Caelo	Cloreto de metacolina	162293	22635	40	20160815*
Caelo	Cloreto de metacolina	16229304	22661	40	20160815
Caelo	Cloreto de metacolina	16229301	22662	40	20160815
Euro OTC	Cloreto de metacolina	2001028	25249	40	20200720*
Fagron	Cloreto de metacolina	12F01-N04	20733	60	1403251
Fagron	Cloreto de metacolina	16L20-B01-329966	22976	40	20170123
Fagron	Cloreto de metacolina	16L20-B01-329968	22977	40	20170123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 520 spectra of 11 reference samples from the substance/substance group *Cloreto de metacolina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 442 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Cloreto de metacolina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloreto de metacolina	163299	23049	40
Caelo	Cloreto de metacolina	20003216002	26304	30
Caelo	Cloreto de metacolina	23000519	26726	40
Fagron	Cloreto de metacolina	17H03-B02-346564	24287	40
Fagron	Cloreto de metacolina	22B07-B22-23069	26823	40
Caelo	Cloreto de metacolina	163299	23624	40
Caelo	Cloreto de metacolina	20003216002	26304SI	20
Caelo	Cloreto de metacolina	23000519	26726SI	20

- 201 814 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 46 spectra from 23 *Apo-Ident* customers from 32 batches from the substance/substance group *Cloreto de metacolina*.

- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
anzag 18.12.14 25,19	Cloreto de metacolina	14G30-B03-296209	1
Caelo	Cloreto de metacolina	16329901	2
Caelo	Cloreto de metacolina	17D13-B04-334377	1
Caelo	Cloreto de metacolina	23000519001	1
Caesar & Loretz GmbH...	Cloreto de metacolina	23000519003	1
Euro OTC	Cloreto de metacolina	2001028-01	1
Fagron	Cloreto de metacolina	10031504	1
Fagron	Cloreto de metacolina	13/13-N03	2
Fagron	Cloreto de metacolina	13121712	1
Fagron	Cloreto de metacolina	13G10-N05	1
Fagron	Cloreto de metacolina	14G30-B03-296210	1
Fagron	Cloreto de metacolina	14K20-B03-300973	2
Fagron	Cloreto de metacolina	15F10-B02-312160	1
Fagron	Cloreto de metacolina	15F10-B02-315523	1
Fagron	Cloreto de metacolina	15F10-B02-315831	1
Fagron	Cloreto de metacolina	160004A	1
Fagron	Cloreto de metacolina	16L20-B01	1
Fagron	Cloreto de metacolina	16L20-B01-329970	1
Fagron	Cloreto de metacolina	17D13-B04	1
Fagron	Cloreto de metacolina	17D13-B04-334377	2
Fagron	Cloreto de metacolina	17D13-B04-334378	1
Fagron	Cloreto de metacolina	17D13-B04-340803	1
Fagron	Cloreto de metacolina	17H03-B02-346563	3
Fagron	Cloreto de metacolina	17h03-b02-346564	1
Fagron	Cloreto de metacolina	17H03-B02-346564	7
Fagron	Cloreto de metacolina	19H07-B04365767	1
Fagron	Cloreto de metacolina	19H07-B04-365768	2
Fagron	Cloreto de metacolina	19H07-B08-365767	1
Fagron	Cloreto de metacolina	24061503	1
Fagron	Cloreto de metacolina	312160	1
Flamma s.p.a	Cloreto de metacolina	14G30-B03-296211	1
Inresa	Cloreto de metacolina	160P02A/09062017	1
Phoenix/Cealo	Cloreto de metacolina	16L20-B01-329968	1

- 236 021 spectra from 1515 *Apo-Ident* customers from a total of 49 226 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloreto de metacolina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloreto de metacolina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	270	0	201 814
Type C	0	46	0	236 021

The substance/substance group *Cloreto de metacolina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.9565 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20733	20733	0,00	211,67
21251	20733	24,46	196,09
21420	25249	86,66	185,92
21590	22635	17,45	205,96
21592	20733	27,17	185,84
22635	22635	0,00	224,30
22661	20733	26,77	199,83
22662	22635	11,02	209,88
22976	20733	7,75	212,64
22977	20733	25,07	203,76
25249	25249	0,00	211,68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de ambroxol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20742-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de ambroxol; Ambroxol, cloridrato; Ambroxoli hydrochloridum

Special notes

When selecting the *Cloridrato de ambroxol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de ambroxol	10	18	176

Second-stage model

For differentiation of the substance/substance group *Cloridrato de ambroxol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de ambroxol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	64,08	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de ambroxol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de ambroxol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de ambroxol	161996	22636	40	20160810*
Caelo	Cloridrato de ambroxol	171582	23344	40	20170607*
Euro OTC	Cloridrato de ambroxol	11110008-01	20742	40	1401146
Euro OTC	Cloridrato de ambroxol	1311032-01	21244	40	20131219
Euro OTC	Cloridrato de ambroxol	1509032	21942	60	20151027*
Euro OTC	Cloridrato de ambroxol	1601008	22298	60	20160119*
Euro OTC	Cloridrato de ambroxol	1602015	22347	60	20160217*
Euro OTC	Cloridrato de ambroxol	1604035	22550	40	20160428*
Fagron	Cloridrato de ambroxol	13I24-N02	21230	40	20131017
Fagron	Cloridrato de ambroxol	19E01-B02-361735	24821	40	20190606

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Cloridrato de ambroxol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 502 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 21 reference samples from the substance/substance group *Cloridrato de ambroxol*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de ambroxol	172860	23801	40
Caelo	Cloridrato de ambroxol	190618	24524	40
Caelo	Cloridrato de ambroxol	22000044	26000	40
Caelo	Cloridrato de ambroxol	23000573	26842	40
Caelo	Cloridrato de ambroxol	23003608	27246	40
Caelo	Cloridrato de ambroxol	24001656	27433	40
Euro OTC	Cloridrato de ambroxol	1609002	22800	40
Euro OTC	Cloridrato de ambroxol	1702004	23155	40
Euro OTC	Cloridrato de ambroxol	1711021	23894	40
Euro OTC	Cloridrato de ambroxol	1806009	24155	40
Euro OTC	Cloridrato de ambroxol	1811039	24423	40
Euro OTC	Cloridrato de ambroxol	1904001	24623	40
Euro OTC	Cloridrato de ambroxol	1911002	24969	40
Euro OTC	Cloridrato de ambroxol	2011004	25463	40
Euro OTC	Cloridrato de ambroxol	2201029	25943	40
Euro OTC	Cloridrato de ambroxol	2210020	26440	40
Euro OTC	Cloridrato de ambroxol	2402033	27289	40
Fagron	Cloridrato de ambroxol	23I29-B08-002374	27414	40
Caelo	Cloridrato de ambroxol	22000044	26000SI	10
Caelo	Cloridrato de ambroxol	23000573	26842SI	20
Euro OTC	Cloridrato de ambroxol	2201029	25943SI	10

- 201 324 spectra from a total of 4027 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1554 spectra from 556 *Apo-Ident* customers from 177 batches from the substance/substance group *Cloridrato de ambroxol*.
- Among them are spectra of independent samples from 176 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de ambroxol	1702004-01	2
	Cloridrato de ambroxol	211020-01	1
	Cloridrato de ambroxol	21I29-B02-215601	1
	Cloridrato de ambroxol	22000044002	4
	Cloridrato de ambroxol	22000044012	1
	Cloridrato de ambroxol	22000044016	6
	Cloridrato de ambroxol	22000044021	17
	Cloridrato de ambroxol	22000044022	1
	Cloridrato de ambroxol	2201029-03	2
	Cloridrato de ambroxol	2210020-01	18
	Cloridrato de ambroxol	2210020-02	6
	Cloridrato de ambroxol	2210020-03	3
	Cloridrato de ambroxol	22J31-B01-224227	1
	Cloridrato de ambroxol	23000573001	4
	Cloridrato de ambroxol	23000573003	12
	Cloridrato de ambroxol	23003608003	5
	Cloridrato de ambroxol	240203301	1
	Cloridrato de ambroxol	AXLO747202207	1
	Cloridrato de ambroxol	CEPABX001L21	1
AHD/EuRho	Cloridrato de ambroxol	2011004-01	1
AHD	Cloridrato de ambroxol	2201029-03	2
AHD	Cloridrato de ambroxol	2210020-01	2
AHD	Cloridrato de ambroxol	2210020-03	1
AHD	Cloridrato de ambroxol	23003608001	3
AHD	Cloridrato de ambroxol	233608001	1
AHD	Cloridrato de ambroxol	2402033-01	2
Alliance Healthcare	Cloridrato de ambroxol	20003999017	1
alliance	Cloridrato de ambroxol	2210020-01	1
Anuh Phama Limited	Cloridrato de ambroxol	2201029-03	1
Anuh Pharma ltd	Cloridrato de ambroxol	2201029-01	1
Anzag	Cloridrato de ambroxol	15G15-B01-316109	1
Anzag	Cloridrato de ambroxol	22000044002	1
Anzag	Cloridrato de ambroxol	2210020-01	4
APO IDENT	Cloridrato de ambroxol	1711021-02	2
APO IDENT	Cloridrato de ambroxol	1806009-01	2
apo-ident	Cloridrato de ambroxol	1806009-01	1
Audor Pharma	Cloridrato de ambroxol	1911002-02	2
Caedo	Cloridrato de ambroxol	192983012	1
Caelo	Cloridrato de ambroxol	1602015-02	1
Caelo	Cloridrato de ambroxol	1609002-01	3
Caelo	Cloridrato de ambroxol	1609002-02	2
Caelo	Cloridrato de ambroxol	16199602	1
Caelo	Cloridrato de ambroxol	16199603	2
Caelo	Cloridrato de ambroxol	16309201	2
Caelo	Cloridrato de ambroxol	17002902	2
Caelo	Cloridrato de ambroxol	17002904	1
Caelo	Cloridrato de ambroxol	17002905	1
Caelo	Cloridrato de ambroxol	1702004-02	4
Caelo	Cloridrato de ambroxol	170522AH/16309201	1
Caelo	Cloridrato de ambroxol	171102101	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de ambroxol	1711021-02	4
Caelo	Cloridrato de ambroxol	17158201	3
Caelo	Cloridrato de ambroxol	17158202	6
Caelo	Cloridrato de ambroxol	17158203	2
Caelo	Cloridrato de ambroxol	17158204	2
Caelo	Cloridrato de ambroxol	17286001	8
Caelo	Cloridrato de ambroxol	1801306	1
Caelo	Cloridrato de ambroxol	18013201	11
Caelo	Cloridrato de ambroxol	18013202	2
Caelo	Cloridrato de ambroxol	18013202/P-23041821	1
Caelo	Cloridrato de ambroxol	18013205	11
Caelo	Cloridrato de ambroxol	18013206	1
Caelo	Cloridrato de ambroxol	18013208	4
Caelo	Cloridrato de ambroxol	18013209	1
Caelo	Cloridrato de ambroxol	18013211	24
Caelo	Cloridrato de ambroxol	18013214	1
Caelo	Cloridrato de ambroxol	18013216	1
Caelo	Cloridrato de ambroxol	18013219	7
Caelo	Cloridrato de ambroxol	18013221	1
Caelo	Cloridrato de ambroxol	1806009-01	1
Caelo	Cloridrato de ambroxol	1811039-01	2
Caelo	Cloridrato de ambroxol	1904001-01	4
Caelo	Cloridrato de ambroxol	19061803	14
Caelo	Cloridrato de ambroxol	19061804	26
Caelo	Cloridrato de ambroxol	19061805	1
Caelo	Cloridrato de ambroxol	19061809	17
Caelo	Cloridrato de ambroxol	19061813	4
Caelo	Cloridrato de ambroxol	19061815	29
Caelo	Cloridrato de ambroxol	1911002-01	4
Caelo	Cloridrato de ambroxol	1911002-02	1
Caelo	Cloridrato de ambroxol	192983001	25
Caelo	Cloridrato de ambroxol	192983002	4
Caelo	Cloridrato de ambroxol	192983003	3
Caelo	Cloridrato de ambroxol	192983006	21
Caelo	Cloridrato de ambroxol	192983008	37
Caelo	Cloridrato de ambroxol	192983011	3
Caelo	Cloridrato de ambroxol	192983012	19
Caelo	Cloridrato de ambroxol	20003996011	1
Caelo	Cloridrato de ambroxol	20003998002	4
Caelo	Cloridrato de ambroxol	20003999002	34
Caelo	Cloridrato de ambroxol	20003999003	25
Caelo	Cloridrato de ambroxol	20003999008	3
Caelo	Cloridrato de ambroxol	20003999011	15
Caelo	Cloridrato de ambroxol	20003999014	2
Caelo	Cloridrato de ambroxol	20003999015	3
Caelo	Cloridrato de ambroxol	20003999017	16
Caelo	Cloridrato de ambroxol	2000399915	1
Caelo	Cloridrato de ambroxol	2011004-01	1
Caelo	Cloridrato de ambroxol	2021904	1
Caelo	Cloridrato de ambroxol	2100086001	1
Caelo	Cloridrato de ambroxol	21001184001	1
Caelo	Cloridrato de ambroxol	210518/1	1
Caelo	Cloridrato de ambroxol	22000044001	2
Caelo	Cloridrato de ambroxol	22000044002	12
Caelo	Cloridrato de ambroxol	22000044003	18
Caelo	Cloridrato de ambroxol	220000440116	1
Caelo	Cloridrato de ambroxol	22000044012	1
Caelo	Cloridrato de ambroxol	22000044016	7
Caelo	Cloridrato de ambroxol	2200044003	1
Caelo	Cloridrato de ambroxol	2200044016	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de ambroxol	2201029-01	1
Caelo	Cloridrato de ambroxol	23000573003	2
Caelo	Cloridrato de ambroxol	26011902	1
Caelo	Cloridrato de ambroxol	27101707	1
Caelo	Cloridrato de ambroxol	AXL0512201612	1
Caeolo/Gehe	Cloridrato de ambroxol	1702004-02	2
Caesar & Loretz GmbH...	Cloridrato de ambroxol	22000044003	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	22000044016	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	20003999011	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	192983008	1
Caesar & Loretz GmbH/AHD	Cloridrato de ambroxol	20003999002	3
Caesar & Loretz GmbH/G	Cloridrato de ambroxol	19061809	3
Caesar & Loretz GmbH/G	Cloridrato de ambroxol	20003999002	1
Caesar & Loretz GmbH/gehe	Cloridrato de ambroxol	19061804	1
Caesar & Loretz GmbH/Gehe	Cloridrato de ambroxol	19061815	1
Caesar & Loretz GmbH/Gehe	Cloridrato de ambroxol	192983012	2
Caesar & Loretz GmbH/Gehe	Cloridrato de ambroxol	20003999002	5
Caesar & Loretz GmbH/Gehe	Cloridrato de ambroxol	20003999011	1
Caesar & Loretz GmbH/Gehe	Cloridrato de ambroxol	22000044002	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	20003999017	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	22000044002	1
Caesar & Loretz GmbH/Kehr	Cloridrato de ambroxol	19061804	1
Caesar & Loretz GmbH/Kehr	Cloridrato de ambroxol	22000044003	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	20003999002	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	20003999017	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	22000044002	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	19061802	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	192983008	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	20003999002	2
Caesar & Loretz GmbH...	Cloridrato de ambroxol	22000044003	1
Caesar & Loretz GmbH...	Cloridrato de ambroxol	20003999015	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	17286001	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	18013205	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	18013211	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	18013219	3
Caesar & Loretz GmbH	Cloridrato de ambroxol	19061803	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	19061804	6
Caesar & Loretz GmbH	Cloridrato de ambroxol	19061805	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	19061809	3
Caesar & Loretz GmbH	Cloridrato de ambroxol	19061815	10
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983001	7
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983002	2
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983003	4
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983006	6
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983008	10
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983010	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983011	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	192983012	6
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003998002	5
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003999002	13
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003999003	10
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003999008	3
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003999011	8
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003999014	3
Caesar & Loretz GmbH	Cloridrato de ambroxol	20003999017	11
Caesar & Loretz GmbH	Cloridrato de ambroxol	21001184001	4
Caesar & Loretz GmbH	Cloridrato de ambroxol	22000044002	6
Caesar & Loretz GmbH	Cloridrato de ambroxol	22000044003	10
Caesar & Loretz GmbH	Cloridrato de ambroxol	22000044012	1
Caesar & Loretz GmbH	Cloridrato de ambroxol	22000044016	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de ambroxol	22000044021	1
Caesar & Loretz	Cloridrato de ambroxol	19061809	1
Cealo/Gehe	Cloridrato de ambroxol	171158204	1
Cealo/Sanacorp	Cloridrato de ambroxol	22000044003	1
Chem & Pharma	Cloridrato de ambroxol	AXL0361201310	1
Ebert & Jacobi	Cloridrato de ambroxol	1806009-01	1
Ensbona/Eimermacher	Cloridrato de ambroxol	1711021-02	1
E-plus	Cloridrato de ambroxol	1711021-02	1
Eu Rho	Cloridrato de ambroxol	1911002-02	1
Eurho / GEHE	Cloridrato de ambroxol	2011004-01	1
EuRho- Phoenix	Cloridrato de ambroxol	2201029-02	1
EuRho/ Anzag	Cloridrato de ambroxol	220504(2201029-01)	1
EuRho/ NOWEDA	Cloridrato de ambroxol	1806009-01	1
EuRho/ NOWEDA	Cloridrato de ambroxol	1811039-01	1
Eurho/AHD	Cloridrato de ambroxol	2011004-01	1
Eurho/Anzag	Cloridrato de ambroxol	1811039-01	1
EuRho/Fiebig	Cloridrato de ambroxol	1811039-01	1
EuRho/Fiebig	Cloridrato de ambroxol	20212004-01	1
EuRho/Gehe	Cloridrato de ambroxol	1911002-02	1
EuRho/Gehe	Cloridrato de ambroxol	2011004-02	1
Eurho/Noweda	Cloridrato de ambroxol	1911002-02	1
EuRho/ph	Cloridrato de ambroxol	1911002-01	1
Eurho/Phoenix	Cloridrato de ambroxol	190400101	1
EuRho	Cloridrato de ambroxol	1602015-02	2
EuRho	Cloridrato de ambroxol	1711021-02	1
EuRho	Cloridrato de ambroxol	1811039-01	1
EuRho	Cloridrato de ambroxol	1911002-01	1
euRho	Cloridrato de ambroxol	1911002-02	1
EuRho	Cloridrato de ambroxol	1911002-02	1
EuRho	Cloridrato de ambroxol	2011001-01	1
EuRho	Cloridrato de ambroxol	2011004-01	1
EuRho	Cloridrato de ambroxol	2011004-03	1
EuRho	Cloridrato de ambroxol	2201029-01	2
EuRho	Cloridrato de ambroxol	2201029-03	2
Euro OCT/	Cloridrato de ambroxol	1904001-01	1
Euro OTC	Cloridrato de ambroxol	1(1806009-01)	1
Euro OTC	Cloridrato de ambroxol	111039-01	1
Euro OTC	Cloridrato de ambroxol	1311032-01	1
Euro OTC	Cloridrato de ambroxol	1509032-01	1
Euro OTC	Cloridrato de ambroxol	1601015-2	1
Euro OTC	Cloridrato de ambroxol	1602015-02	2
Euro OTC	Cloridrato de ambroxol	160215-02	1
Euro OTC	Cloridrato de ambroxol	1604032-01	1
Euro OTC	Cloridrato de ambroxol	1604035-01	3
Euro OTC	Cloridrato de ambroxol	1604035-02	13
Euro OTC	Cloridrato de ambroxol	1609002-01	15
Euro OTC	Cloridrato de ambroxol	1609002-02	21
Euro OTC	Cloridrato de ambroxol	170192	1
Euro OTC	Cloridrato de ambroxol	170200401	1
Euro OTC	Cloridrato de ambroxol	1702004-01	12
Euro OTC	Cloridrato de ambroxol	170200402	1
Euro OTC	Cloridrato de ambroxol	1702004-02	11
Euro OTC	Cloridrato de ambroxol	171102-01	1
Euro OTC	Cloridrato de ambroxol	171102101	1
Euro OTC	Cloridrato de ambroxol	1711021-01	21
Euro OTC	Cloridrato de ambroxol	1711021-01/P-030518	1
Euro OTC	Cloridrato de ambroxol	1711021-02	29
Euro OTC	Cloridrato de ambroxol	1806009	2
Euro OTC	Cloridrato de ambroxol	1806009-01	34
Euro OTC	Cloridrato de ambroxol	1806009-1	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de ambroxol	181103901	3
Euro OTC	Cloridrato de ambroxol	1811039-01	45
Euro OTC	Cloridrato de ambroxol	190400-01	1
Euro OTC	Cloridrato de ambroxol	1904001	2
Euro OTC	Cloridrato de ambroxol	1904001-0	1
Euro OTC	Cloridrato de ambroxol	190400101	2
Euro OTC	Cloridrato de ambroxol	1904001-01	77
Euro OTC	Cloridrato de ambroxol	19040101	1
Euro OTC	Cloridrato de ambroxol	1904401	1
Euro OTC	Cloridrato de ambroxol	191002-01	1
Euro OTC	Cloridrato de ambroxol	191100-01	1
Euro OTC	Cloridrato de ambroxol	19110002-01	1
Euro OTC	Cloridrato de ambroxol	1911001-01	1
Euro OTC	Cloridrato de ambroxol	1911001-02	1
Euro OTC	Cloridrato de ambroxol	191100201	2
Euro OTC	Cloridrato de ambroxol	1911002-01	45
Euro OTC	Cloridrato de ambroxol	191100202	1
Euro OTC	Cloridrato de ambroxol	1911002-02	41
Euro OTC	Cloridrato de ambroxol	1911002-42	1
Euro OTC	Cloridrato de ambroxol	1911008-04	1
Euro OTC	Cloridrato de ambroxol	191102-02	2
Euro OTC	Cloridrato de ambroxol	1911022-01	1
Euro OTC	Cloridrato de ambroxol	1L2001	1
Euro OTC	Cloridrato de ambroxol	2(1904001-01)	1
Euro OTC	Cloridrato de ambroxol	201100401	2
Euro OTC	Cloridrato de ambroxol	2011004-01	71
Euro OTC	Cloridrato de ambroxol	2011004-02	13
Euro OTC	Cloridrato de ambroxol	2011004-03	10
Euro OTC	Cloridrato de ambroxol	2011004-04	1
Euro OTC	Cloridrato de ambroxol	201104-01	1
Euro OTC	Cloridrato de ambroxol	201104-03	1
Euro OTC	Cloridrato de ambroxol	220102901	1
Euro OTC	Cloridrato de ambroxol	2201029-01	42
Euro OTC	Cloridrato de ambroxol	2201029-02	9
Euro OTC	Cloridrato de ambroxol	2201029-03	7
Euro OTC	Cloridrato de ambroxol	220109-02	1
Euro OTC	Cloridrato de ambroxol	220715(2201029-01)	1
Euro OTC	Cloridrato de ambroxol	2210020-01	6
Euro OTC	Cloridrato de ambroxol	2210020-02	2
Euro OTC	Cloridrato de ambroxol	27061702	1
Euro OTC	Cloridrato de ambroxol	3111805	1
Euro OTC	Cloridrato de ambroxol	811030-01	1
Euro OTC	Cloridrato de ambroxol	axl0492201608	1
Euro OTC	Cloridrato de ambroxol	AXL056201709	1
Euro OTC	Cloridrato de ambroxol	AXL0592201803	2
Euro OTC	Cloridrato de ambroxol	AXL0601201807	1
Euro OTC	Cloridrato de ambroxol	CEPABIX001L21	1
Euro/Noweda	Cloridrato de ambroxol	1509032-01	1
Euro/Noweda	Cloridrato de ambroxol	181103901	1
Euro/Phönix	Cloridrato de ambroxol	1904001-01	1
Euro/Phönix	Cloridrato de ambroxol	2201029-01	2
Euroo/Gehe	Cloridrato de ambroxol	1702004-02	1
EuroTOC	Cloridrato de ambroxol	1602015-01	1
EurRho	Cloridrato de ambroxol	2011004-01	1
Fagron	Cloridrato de ambroxol	12K12-N02	1
Fagron	Cloridrato de ambroxol	1602015-01	1
Fagron	Cloridrato de ambroxol	16G12-B06-326184	1
Fagron	Cloridrato de ambroxol	16G12-B06-333330	2
Fagron	Cloridrato de ambroxol	17K30-B04-352348	1
Fiebig	Cloridrato de ambroxol	1911002-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gatt-Koller	Cloridrato de ambroxol	180600901	1
Gatt-Koller	Cloridrato de ambroxol	181103901	2
Gehe amax	Cloridrato de ambroxol	1904001-01	1
Gehe	Cloridrato de ambroxol	16199602	1
GEHE	Cloridrato de ambroxol	1702004-02	1
GEHE	Cloridrato de ambroxol	1711021-01	1
Gehe	Cloridrato de ambroxol	18013211	1
GEHE	Cloridrato de ambroxol	1904001-01	3
Gehe	Cloridrato de ambroxol	19061804	2
Gehe	Cloridrato de ambroxol	1911002-01	3
Gehe	Cloridrato de ambroxol	192983001	1
Gehe	Cloridrato de ambroxol	20003999002	1
Gehe	Cloridrato de ambroxol	20003999011	1
Gehe	Cloridrato de ambroxol	2011004	1
Gehe	Cloridrato de ambroxol	2011004-02	3
Gehe	Cloridrato de ambroxol	22000044002	1
Gehe	Cloridrato de ambroxol	22000044020	5
Gehe	Cloridrato de ambroxol	2200044020	1
Gehe	Cloridrato de ambroxol	2201029-01	1
Gehe	Cloridrato de ambroxol	2300057001	1
Gehe	Cloridrato de ambroxol	23000573001	2
Gehe	Cloridrato de ambroxol	23000573002	1
Hanse/Sanacorp	Cloridrato de ambroxol	22000044001	1
Jenne	Cloridrato de ambroxol	2210020-01	2
Jenne	Cloridrato de ambroxol	2210020-02	4
Jenne	Cloridrato de ambroxol	23003608002	2
Kehr	Cloridrato de ambroxol	18013201	1
Midas	Cloridrato de ambroxol	2011004-01	1
Noweda 23.07.2019	Cloridrato de ambroxol	19061804	1
Noweda Taucha	Cloridrato de ambroxol	2011004-03	2
Noweda/ Caesar&Loren…	Cloridrato de ambroxol	192983001	1
Noweda/EuRo	Cloridrato de ambroxol	1609002-02	1
Noweda	Cloridrato de ambroxol	1711021-01	1
Noweda	Cloridrato de ambroxol	17158201	2
Noweda	Cloridrato de ambroxol	19061804	1
Noweda	Cloridrato de ambroxol	1911002-02	1
Noweda	Cloridrato de ambroxol	192983012	1
Noweda	Cloridrato de ambroxol	20003999002	2
Noweda	Cloridrato de ambroxol	20003999011	1
Noweda	Cloridrato de ambroxol	20003999017	1
Noweda	Cloridrato de ambroxol	21001184001	1
Noweda	Cloridrato de ambroxol	22000044016	1
Noweda	Cloridrato de ambroxol	22000044021	1
Noweda	Cloridrato de ambroxol	2210020-02	1
Noweda	Cloridrato de ambroxol	AXL0747202207	1
phoenix /eurho	Cloridrato de ambroxol	1911002-01	1
Phoenix 09.10.2017	Cloridrato de ambroxol	1702004-02	2
Phoenix 21.6.2019, 17,35EUR	Cloridrato de ambroxol	1811039-01	1
Phoenix	Cloridrato de ambroxol	1604035-02	1
Phoenix	Cloridrato de ambroxol	200003999011	1
Phoenix	Cloridrato de ambroxol	20003999017	1
Phoenix	Cloridrato de ambroxol	22000044016	1
Phoenix	Cloridrato de ambroxol	3188	1
Phoenix	Cloridrato de ambroxol	3198	1
PHÖNIX	Cloridrato de ambroxol	1702004-01	1
Phönix	Cloridrato de ambroxol	1904001-01	1
Phönix	Cloridrato de ambroxol	22000044002	1
Phönix	Cloridrato de ambroxol	22000044003	1
Phönix	Cloridrato de ambroxol	AXL0747202207	1
Sana/Hanse	Cloridrato de ambroxol	23003608002	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp EURO	Cloridrato de ambroxol	1806009-01	1
Sanacorp/EuRho	Cloridrato de ambroxol	1806009-01	3
Sanacorp/EuRho	Cloridrato de ambroxol	1904001-01	1
Sanacorp	Cloridrato de ambroxol	170204-02	1
Sanacorp	Cloridrato de ambroxol	1711021-01	2
Sanacorp	Cloridrato de ambroxol	18013219	2
SANACORP	Cloridrato de ambroxol	1811039-01	2
SANACORP	Cloridrato de ambroxol	19061802	1
Sanacorp	Cloridrato de ambroxol	19061815	5
Sanacorp	Cloridrato de ambroxol	1911002-01	1
Sanacorp	Cloridrato de ambroxol	192983001	2
Sanacorp	Cloridrato de ambroxol	20003999003	1
Sanacorp	Cloridrato de ambroxol	21001184001	1
Sanacorp	Cloridrato de ambroxol	22000044002	1
Sanacorp	Cloridrato de ambroxol	22000044015	1
Sanacorp	Cloridrato de ambroxol	22000044016	1
Sanacorp	Cloridrato de ambroxol	22000044021	3
Sanacorp	Cloridrato de ambroxol	2201029-01	1
Sanacorp	Cloridrato de ambroxol	2201029-02	1
Sanacorp	Cloridrato de ambroxol	2201029-03	1
Sanacorp	Cloridrato de ambroxol	23003608002	3
Sanacorp	Cloridrato de ambroxol	720220007	1
synthetisch	Cloridrato de ambroxol	2201029-01	2
Ven Petro	Cloridrato de ambroxol	1911002-01	1
Ven Petrochem&Pharma…	Cloridrato de ambroxol	18013205	1
Ven Petrochem&Pharma/Gehe	Cloridrato de ambroxol	18013211	2
Ven Petro-Chem	Cloridrato de ambroxol	1806009-01	1

- 234 513 spectra from 1515 *Apo-Ident* customers from a total of 49 089 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de ambroxol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de ambroxol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	760	0	201 324
Type C	0	1542	12	234 513

The substance/substance group *Cloridrato de ambroxol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	99.2278 % (> 99.0347 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20742	20742	0,00	125,26
21230	21942	10,96	143,97
21244	22550	5,90	133,87
21942	21942	0,00	144,24
22298	22298	0,00	134,21
22347	22347	0,00	131,07
22550	22550	0,00	131,73
22636	22636	0,00	126,61
23344	23344	0,00	130,08
24821	21942	11,06	145,00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de amilorida di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21879-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de amilorida di-hidratado; Amilorida, cloridrato di-hidratado; Amiloridi hydrochloridum dihydricum

Special notes

When selecting the *Cloridrato de amilorida di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de amilorida di-hidratado	5	3	9

Second-stage model

For differentiation of the substance/substance group *Cloridrato de amilorida di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de amilorida di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	102,26	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de amilorida di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de amilorida di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de amilorida d…	13J08-B04-288620	21879	60	AR-16-FG-008919-01
Fagron	Cloridrato de amilorida d…	13J08-B04-304547	22339	60	20131024
Fagron	Cloridrato de amilorida d…	17F02-B06-335953	23525	40	20170630
Fagron	Cloridrato de amilorida d…	23E30-B10-229440	26985	40	20230624
Fagron	Cloridrato de amilorida d…	23E30-B10-229440	26985SI	20	20230624
Fagron	Cloridrato de amilorida d…	23L12-B13-235070	27168	40	20240123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Cloridrato de amilorida di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 702 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Cloridrato de amilorida di-hidratado*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de amilorida d…	15C25-B05-325653	22834	40
Fagron	Cloridrato de amilorida d…	16K07-B02-329114	23119	40
Fagron	Cloridrato de amilorida d…	21D20-F01-379327	25904	40
Fagron	Cloridrato de amilorida d…	21D20-F01-379327	25904SI	10
Fagron	Cloridrato de amilorida d…	23L12-B13-235070	27168SI†	20

- 201 934 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 10 spectra from 4 *Apo-Ident* customers from 9 batches from the substance/substance group *Cloridrato de amilorida di-hidratado*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Ebert 04.04.2014	Cloridrato de amilorida d…	13J08-B04	1
Fagron	Cloridrato de amilorida d…	17J02-B04	1
Fagron	Cloridrato de amilorida d…	17J02-B04-341175	2
Fagron	Cloridrato de amilorida d…	18C08-B03-353047	1
Fagron	Cloridrato de amilorida d…	18K16-B01-360014	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de amilorida d…	20h25-f03-373607	1
Fagron	Cloridrato de amilorida d…	3100/07/15	1
Fagron	Cloridrato de amilorida d…	3100-03-12	1
Fagron	Cloridrato de amilorida d…	3100-07-15	1

- 236 057 spectra from 1515 *Apo-Ident* customers from a total of 49 249 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de amilorida di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de amilorida di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	150	0	201 934
Type C	0	10	0	236 057

The substance/substance group *Cloridrato de amilorida di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21879	21879	0,00	142,84
22339	21879	5,38	143,13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23525	21879	48,91	148,18
26985	21879	28,98	141,52
27168	21879	20,83	142,33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de amitriptilina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22844-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de amitriptilina; Amitriptilina, cloridrato; Amitriptylini hydrochloridum

Special notes

When selecting the *Cloridrato de amitriptilina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de amitriptilina	6	3	77

Second-stage model

For differentiation of the substance/substance group *Cloridrato de amitriptilina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de amitriptilina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de doxepina	98,43	–
⋮	⋮	⋮
Acetato de ciproterona	>50	72,24
Prednicarbato	>50	124,95
Cloridrato de oxibutinina	>50	127,20
Levocarnitina	>50	191,23
Capsaicina	>50	218,53
Tetracaína	>50	228,57
Citrato de sódio	>50	237,42
Valina	>50	323,99
Metoxisaleno	>50	351,19
Acetato de noretisterona	>50	427,43
Piridoxal-5-fosfato	>50	442,31
Alfaestradiol	>50	467,04
Cloridrato de quinina di-hidratado	>50	539,42
Cloridrato de ciprofloxacina	>50	596,95
Heparina sódica	>50	639,33
Triclosan	>50	1736,38
Amifampridina	>50	2330,42
Sacarose	>50	2609,06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de amitriptilina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de amitriptilina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de amitriptilina	16C31-B01-325540	22844	40	20160425
Fagron	Cloridrato de amitriptilina	18A16-B06-348643	24180	40	1909242

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de amitriptilina	21G23-B03-213920	25842	50	20210906
Fagron	Cloridrato de amitriptilina	23C04-B07-227329	26663	30	20230327
Inresa	Cloridrato de amitriptilina	005669/17112016	22845	40	1705099
Inresa	Cloridrato de amitriptilina	005669/06022017	23078	40	20160524

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Cloridrato de amitriptilina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 722 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 6 reference samples from the substance/substance group *Cloridrato de amitriptilina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de amitriptilina	17E11-B02-335098	23528	40
Fagron	Cloridrato de amitriptilina	19C08-B02-362280	24689	40
Fagron	Cloridrato de amitriptilina	22F28-B04-222454	26282	40
Fagron	Cloridrato de amitriptilina	21G23-B03-213920	25842SI†	10
Fagron	Cloridrato de amitriptilina	22F28-B04-222454	26282SI	20
Fagron	Cloridrato de amitriptilina	23C04-B07-227329	26663SI†	20

- 201 914 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples

are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 239 spectra from 107 *Apo-Ident* customers from 85 batches from the substance/substance group *Cloridrato de amitriptilina*.
- Among them are spectra of independent samples from 75 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de amitriptilina		1
	Cloridrato de amitriptilina	2113440	1
	Cloridrato de amitriptilina	22B10-B04	1
	Cloridrato de amitriptilina	22B10-B04-217981	3
	Cloridrato de amitriptilina	2301192	1
	Cloridrato de amitriptilina	23C04-B07-227328	6
	Cloridrato de amitriptilina	23C04-B07-227329	2
	Cloridrato de amitriptilina	23C04-B07-231756	1
	Cloridrato de amitriptilina	23C04-B07-227329	1
	Cloridrato de amitriptilina	B07-2317506	11
	Cloridrato de amitriptilina	B09-2361602	1
AEP	Cloridrato de amitriptilina	23C04-B07-231756	1
Alliance Healthcare	Cloridrato de amitriptilina	23C04-B07-227329	1
Alliance Healthcare	Cloridrato de amitriptilina	23C04-B07-231756	1
Caelo	Cloridrato de amitriptilina	19C08-b02-368626	1
Caelo	Cloridrato de amitriptilina	22B10B04217981	1
Euro OTC	Cloridrato de amitriptilina		1
Euro OTC	Cloridrato de amitriptilina	1019Q-03993	1
Euro OTC	Cloridrato de amitriptilina	1506024	2
Euro OTC	Cloridrato de amitriptilina	19C08-B02-362280	1
Euro OTC	Cloridrato de amitriptilina	2715E-07209	1
Fagron	Cloridrato de amitriptilina	1(1901746)	1
Fagron	Cloridrato de amitriptilina	12496176	1
Fagron	Cloridrato de amitriptilina	12C29-B03-211252	1
Fagron	Cloridrato de amitriptilina	17E-11-B02-335096	1
Fagron	Cloridrato de amitriptilina	17E11-B02-337699	1
Fagron	Cloridrato de amitriptilina	17E11-B02-340187	3
Fagron	Cloridrato de amitriptilina	18A16-B06	2
Fagron	Cloridrato de amitriptilina	18A16-B06-344853	3
Fagron	Cloridrato de amitriptilina	18A16-B06-348642	4
Fagron	Cloridrato de amitriptilina	18A16-B06-348643	2
Fagron	Cloridrato de amitriptilina	18A16-B06-353064	1
Fagron	Cloridrato de amitriptilina	18A16-B06-353065	2
Fagron	Cloridrato de amitriptilina	18A16-B06_346046	1
Fagron	Cloridrato de amitriptilina	1901746	5
Fagron	Cloridrato de amitriptilina	19c08-802-368627	1
Fagron	Cloridrato de amitriptilina	19c08-802372547	1
Fagron	Cloridrato de amitriptilina	19c08-b02	1
Fagron	Cloridrato de amitriptilina	19c08-B02	1
Fagron	Cloridrato de amitriptilina	19C08-B02	8
Fagron	Cloridrato de amitriptilina	19C08-B02-362279	3
Fagron	Cloridrato de amitriptilina	19C08-B02-362280	4
Fagron	Cloridrato de amitriptilina	19C-08-B02-362280	1
Fagron	Cloridrato de amitriptilina	19C08-B02-362281	4

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de amitriptilina	19C08-B02-363377	1
Fagron	Cloridrato de amitriptilina	19C08-B02-363378	5
Fagron	Cloridrato de amitriptilina	19C08-B02-365573	1
Fagron	Cloridrato de amitriptilina	19C08-B02-365574	5
Fagron	Cloridrato de amitriptilina	19C08-B02-367679	2
Fagron	Cloridrato de amitriptilina	19C08-B02-3686207	1
Fagron	Cloridrato de amitriptilina	19C08-B02-368627	7
Fagron	Cloridrato de amitriptilina	19C08-B02-370336	6
Fagron	Cloridrato de amitriptilina	19C08-B02-372647	6
Fagron	Cloridrato de amitriptilina	19C08-B02-374309	4
Fagron	Cloridrato de amitriptilina	19C08-B02-370336	1
Fagron	Cloridrato de amitriptilina	2012315	1
Fagron	Cloridrato de amitriptilina	2012436	4
Fagron	Cloridrato de amitriptilina	21C29-803	1
Fagron	Cloridrato de amitriptilina	21C29-B03	4
Fagron	Cloridrato de amitriptilina	21C29-B03-211251	1
Fagron	Cloridrato de amitriptilina	21C29-B03-211252	6
Fagron	Cloridrato de amitriptilina	21G23-B03	2
Fagron	Cloridrato de amitriptilina	21G23-B03-213919	1
Fagron	Cloridrato de amitriptilina	21G23-B03-21392	1
Fagron	Cloridrato de amitriptilina	21G23B03213920	1
Fagron	Cloridrato de amitriptilina	21G23-B03-213920	12
Fagron	Cloridrato de amitriptilina	22810-804-217981	1
Fagron	Cloridrato de amitriptilina	22B10-B04	6
Fagron	Cloridrato de amitriptilina	22B10-B04-2113440	1
Fagron	Cloridrato de amitriptilina	22b10-b04-21791	1
Fagron	Cloridrato de amitriptilina	22B10-B04-217981	24
Fagron	Cloridrato de amitriptilina	22B10-B04-2179891	1
Fagron	Cloridrato de amitriptilina	22B10-B04-218072	3
Fagron	Cloridrato de amitriptilina	22B10-B04-217981	1
Fagron	Cloridrato de amitriptilina	2301192	3
Fagron	Cloridrato de amitriptilina	2-36862007	1
Fagron	Cloridrato de amitriptilina	23C04-B07-227329	1
Fagron	Cloridrato de amitriptilina	B02-3686207	1
Fagron	Cloridrato de amitriptilina	B02-3703306	1
Fagron	Cloridrato de amitriptilina	B03-2112502	2
Fagron	Cloridrato de amitriptilina	B03-2139109	1
Fagron	Cloridrato de amitriptilina	B03-2139200	1
Fagron	Cloridrato de amitriptilina	BO3-2139200	1
Fagron	Cloridrato de amitriptilina	Fagron	1
Fischar/Gehe	Cloridrato de amitriptilina	B03-2112502	1
Fragon Gehe	Cloridrato de amitriptilina	22B10-B04-217981	1
Fragon/Sanacorp	Cloridrato de amitriptilina	1901746	1
Gehe Rostock	Cloridrato de amitriptilina	19C08-B02	2
Gehe Rostock	Cloridrato de amitriptilina	22B10-B04-217981	2
GEHE	Cloridrato de amitriptilina	17E11-B02	1
Gehe	Cloridrato de amitriptilina	19C08-B02-368627	1
Gehe	Cloridrato de amitriptilina	21C29-B03-211252	1
Gehe	Cloridrato de amitriptilina	23C04-B07-231756	1
INRESA/INRESA	Cloridrato de amitriptilina		1
Inresa	Cloridrato de amitriptilina	17112016/P-17031721	1
Inresa	Cloridrato de amitriptilina	5945/12102017	1
Inresa	Cloridrato de amitriptilina	5945/13122017	1
jenne	Cloridrato de amitriptilina	23c04-b07-231756	1
Kehr	Cloridrato de amitriptilina	23C04-B07-227329	1
Kehr	Cloridrato de amitriptilina	23C04-Bo7-227329	1
Kehr	Cloridrato de amitriptilina	23C04-B07-227329	1
Noweda	Cloridrato de amitriptilina	22B10-B04-217981	1
SANACORP	Cloridrato de amitriptilina	19C08-B02	1
Sanacorp	Cloridrato de amitriptilina	22b10-b04-217981	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Cloridrato de amitriptilina	23C04-B07-227329	1

- 235 828 spectra from 1515 *Apo-Ident* customers from a total of 49 175 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de amitriptilina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de amitriptilina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	170	0	201 914
Type C	0	239	0	235 828

The substance/substance group *Cloridrato de amitriptilina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.4895 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22844	24180	10,34	158,86
22845	22845	0,00	152,21
23078	22845	3,81	150,77
24180	24180	0,00	163,32
25842	24180	13,44	166,71
26663	22845	9,95	163,82

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de arginina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20657-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de arginina; Arginina, cloridrato

Special notes

When selecting the *Cloridrato de arginina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de arginina	8	8	24

Second-stage model

For differentiation of the substance/substance group *Cloridrato de arginina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de arginina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	83,16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de arginina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de arginina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de arginina	1306023-01	21776	60	AR-15-FG-008412-01
Euro OTC	Cloridrato de arginina	1603033	22512	40	20160425*
Euro OTC	Cloridrato de arginina	1610042	22877	40	20161128*
Euro OTC	Cloridrato de arginina	1904014	24628	40	20190509*
Euro OTC	Cloridrato de arginina	2008024	25338	40	20200909*
Euro OTC	Cloridrato de arginina	2105005	25673	40	20210531*
Euro OTC	Cloridrato de arginina	2206021	26424	40	20221206*
Fagron	Cloridrato de arginina	22B28-B04-220548	26163	40	20220602
Fagron	Cloridrato de arginina	22B28-B04-220548	26163SI	20	20220602

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Cloridrato de arginina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 350 spectra of 10 reference samples from the substance/substance group *Cloridrato de arginina*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de arginina	1711014	23875	40
Euro OTC	Cloridrato de arginina	1809012	24313	40
Euro OTC	Cloridrato de arginina	1909026	24937	40
Euro OTC	Cloridrato de arginina	2004004	25141	40
Euro OTC	Cloridrato de arginina	2011006	25460	40
Euro OTC	Cloridrato de arginina	2201019	25922	40
Euro OTC	Cloridrato de arginina	2402022	27147	40
Fagron	Cloridrato de arginina	24A10-B09-236592	27179	40
Euro OTC	Cloridrato de arginina	2201019	25922SI	10
Euro OTC	Cloridrato de arginina	2402022	27147SI	20

- 201 734 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 51 spectra from 11 *Apo-Ident* customers from 26 batches from the substance/substance group *Cloridrato de arginina*.

- Among them are spectra of independent samples from 24 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
EuRho	Cloridrato de arginina	1306023-01	1
Euro OTC	Cloridrato de arginina	1306023-01	1
Euro OTC	Cloridrato de arginina	1603033-01	1
Euro OTC	Cloridrato de arginina	1610042-01	1
Euro OTC	Cloridrato de arginina	1610042-02	1
Euro OTC	Cloridrato de arginina	1711014-01	2
Euro OTC	Cloridrato de arginina	1909026-01	1
Euro OTC	Cloridrato de arginina	2004004-01	2
Euro OTC	Cloridrato de arginina	2008024-01	1
Euro OTC	Cloridrato de arginina	2011006-01	2
Euro OTC	Cloridrato de arginina	21011967	1
Euro OTC	Cloridrato de arginina	2105005-01	8
Euro OTC	Cloridrato de arginina	2105005-02	2
Euro OTC	Cloridrato de arginina	2201019-01	6
Euro OTC	Cloridrato de arginina	2202019-01	1
Euro OTC	Cloridrato de arginina	L1212009-01	3
Euro OTC	Cloridrato de arginina	L1407040-01	1
Euro OTC	Cloridrato de arginina	L1407040-02	3
Euro OTC	Cloridrato de arginina	L1506023-01	3
Fagron	Cloridrato de arginina	12C20-N08	1
Fagron	Cloridrato de arginina	13J28-B03	2
Fagron	Cloridrato de arginina	13J28-B03-287766	1
Fagron	Cloridrato de arginina	13j28-b03-287768	1
Fagron	Cloridrato de arginina	13j28-B03-287768	1
Fagron	Cloridrato de arginina	13J28-B032x	1
Hirundo Products Ver…	Cloridrato de arginina	6412784-152	2
Pure encapsulations	Cloridrato de arginina	50152421	1

- 236 016 spectra from 1515 *Apo-Ident* customers from a total of 49 232 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de arginina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de arginina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	350	0	201 734
Type C	0	51	0	236 016

The substance/substance group *Cloridrato de arginina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 88.2353 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21776	21776	0,00	179,78
22512	22512	0,00	180,90
22877	22877	0,00	181,93
24628	24628	0,00	182,13
25338	25338	0,00	183,06
25673	25673	0,00	182,01
26163	22877	7,44	181,78
26424	26424	0,00	177,69

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de benzidamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20624-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de benzidamina; Benzidamina, cloridrato; Benzydamini hydrochloridum

Special notes

When selecting the *Cloridrato de benzidamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de benzidamina	6	7	89

Second-stage model

For differentiation of the substance/substance group *Cloridrato de benzidamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de benzidamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de doxepina	59,69	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de benzidamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de benzidamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Cloridrato de benzidamina	AP300111801004B	24411	40	20180418
Euro OTC	Cloridrato de benzidamina	2011014	25596	40	20210310*
Euro OTC	Cloridrato de benzidamina	2011014-01	25781	50	20210317
Fagron	Cloridrato de benzidamina	14I30-B04-300713	21699	45	AR-15-FG-015977-01
Fagron	Cloridrato de benzidamina	15I17-B02-315060	22268	60	20151211
Fagron	Cloridrato de benzidamina	20K16-F04-375883	25718	50	20210105

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 285 spectra of 6 reference samples from the substance/substance group *Cloridrato de benzidamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 677 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 370 spectra of 11 reference samples from the substance/substance group *Cloridrato de benzidamina*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de benzidamina	2201027	25967	40
Euro OTC	Cloridrato de benzidamina	2301015	26587	40
Euro OTC	Cloridrato de benzidamina	2401026	27372	40
Euro OTC	Cloridrato de benzidamina	2409005	27387	40
Fagron	Cloridrato de benzidamina	16D05-B50-332333	23203	40
Fagron	Cloridrato de benzidamina	17H01-B03-345050	23942	40
Fagron	Cloridrato de benzidamina	18H29-B02-355663	24445	40
Euro OTC	Cloridrato de benzidamina	2201027	25967SI	10
Euro OTC	Cloridrato de benzidamina	2301015	26587SI	20
Euro OTC	Cloridrato de benzidamina	2401026	27372SI	20
Fagron	Cloridrato de benzidamina	16D05-B50-332333	23204	40

- 201 714 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 242 spectra from 195 *Apo-Ident* customers from 96 batches from the substance/substance group *Cloridrato de benzidamina*.

- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de benzidamina	2103302P	1
	Cloridrato de benzidamina	21G10-B09-213933	1
	Cloridrato de benzidamina	21G10-B10-213932	2
	Cloridrato de benzidamina	21G10B10219520	1
	Cloridrato de benzidamina	21G10-B10-219520	3
	Cloridrato de benzidamina	2201027-01	1
	Cloridrato de benzidamina	2201027-02	3
20E13-F02_373489	Cloridrato de benzidamina	Fagron	1
Anzag/ Audov	Cloridrato de benzidamina	AP300111801004B	1
Audor Pharma	Cloridrato de benzidamina	19K25-F01	1
Audor Pharma	Cloridrato de benzidamina	300111702007	1
Audor Pharma	Cloridrato de benzidamina	300111702007b	1
Audor Pharma	Cloridrato de benzidamina	300111702007B	1
Audor Pharma	Cloridrato de benzidamina	300111801004B	3
Audor Pharma	Cloridrato de benzidamina	AP3000111801004B	1
Audor Pharma	Cloridrato de benzidamina	AP300111702007	1
Audor Pharma	Cloridrato de benzidamina	AP300111702007B	6
Audor Pharma	Cloridrato de benzidamina	AP300111801004	1
Audor Pharma	Cloridrato de benzidamina	AP300111801004B	6
Bal Pharma	Cloridrato de benzidamina	AP300111801004B	1
Caelo	Cloridrato de benzidamina	12K07-N16	1
Caelo	Cloridrato de benzidamina	17H01-B03-345050	2
Caelo	Cloridrato de benzidamina	1803309P	1
Caelo	Cloridrato de benzidamina	18H29B02355663	1
Caelo	Cloridrato de benzidamina	18H29B02-358710	1
Caelo	Cloridrato de benzidamina	18H29-B02-358710	2
Caelo	Cloridrato de benzidamina	1903303P	1
Centaur / Gehe	Cloridrato de benzidamina	18H29-B02-361603	1
Euro OTC	Cloridrato de benzidamina	2001026-01	1
Euro OTC	Cloridrato de benzidamina	2011014-01	1
Fagron	Cloridrato de benzidamina		1
Fagron	Cloridrato de benzidamina	12C20-N02	1
Fagron	Cloridrato de benzidamina	12J10-N03	1
Fagron	Cloridrato de benzidamina	12K07-N16	1
Fagron	Cloridrato de benzidamina	13A15-N03	1
Fagron	Cloridrato de benzidamina	13H19_N06	1
Fagron	Cloridrato de benzidamina	13H19-N06	1
Fagron	Cloridrato de benzidamina	14B25-B01-294054	1
Fagron	Cloridrato de benzidamina	1503309P	1
Fagron	Cloridrato de benzidamina	1503313P	1
Fagron	Cloridrato de benzidamina	1503315P	1
Fagron	Cloridrato de benzidamina	15A14-B05	2
Fagron	Cloridrato de benzidamina	15A14-B05-303068	1
Fagron	Cloridrato de benzidamina	15A14-B05-307102	1
Fagron	Cloridrato de benzidamina	15A14-B05-307103	1
Fagron	Cloridrato de benzidamina	15I17-B02	1
Fagron	Cloridrato de benzidamina	16B09-B05-318272	3
Fagron	Cloridrato de benzidamina	16B09-B05-318273	2
Fagron	Cloridrato de benzidamina	16B09-B05-320007	1
Fagron	Cloridrato de benzidamina	16d05-b50-332333	1
Fagron	Cloridrato de benzidamina	16D05-B50-332333	1
Fagron	Cloridrato de benzidamina	16D05-b50-332334	1
Fagron	Cloridrato de benzidamina	16D05-B50-332334	3
Fagron	Cloridrato de benzidamina	1703305P	1
Fagron	Cloridrato de benzidamina	17H01-B03	1
Fagron	Cloridrato de benzidamina	17H01-B03_34641	1
Fagron	Cloridrato de benzidamina	17H01-B03-345050	5
Fagron	Cloridrato de benzidamina	17H01-B03-345051	2
Fagron	Cloridrato de benzidamina	17H01-B03-348469	4
Fagron	Cloridrato de benzidamina	17H01-B03-348470	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de benzidamina	1803309P	4
Fagron	Cloridrato de benzidamina	18H29-02-358710	1
Fagron	Cloridrato de benzidamina	18H29-B02	2
Fagron	Cloridrato de benzidamina	18H29-B02-354329	5
Fagron	Cloridrato de benzidamina	18H29-B02-354330	2
Fagron	Cloridrato de benzidamina	18H29-B02-355318	1
Fagron	Cloridrato de benzidamina	18H29-B02-355663	4
Fagron	Cloridrato de benzidamina	18H29-B02-357424	1
Fagron	Cloridrato de benzidamina	18H29-B02-358710	4
Fagron	Cloridrato de benzidamina	18H29-B02-358711	1
Fagron	Cloridrato de benzidamina	18H29-B02-361603	3
Fagron	Cloridrato de benzidamina	18H29-B-357424	1
Fagron	Cloridrato de benzidamina	1903303P	2
Fagron	Cloridrato de benzidamina	19K25-F01	3
Fagron	Cloridrato de benzidamina	19K25-F01_366695	1
Fagron	Cloridrato de benzidamina	19K25-F01-366695	10
Fagron	Cloridrato de benzidamina	19K25-F01-366697	2
Fagron	Cloridrato de benzidamina	19K25-F01-366699	6
Fagron	Cloridrato de benzidamina	19K25-FO1-366695	1
Fagron	Cloridrato de benzidamina	19K25-FO1-366699	1
Fagron	Cloridrato de benzidamina	2003305P	3
Fagron	Cloridrato de benzidamina	200330SP	1
Fagron	Cloridrato de benzidamina	2003311P	2
Fagron	Cloridrato de benzidamina	20E13-F02	9
Fagron	Cloridrato de benzidamina	20E13-F02-2373489	1
Fagron	Cloridrato de benzidamina	20E13-F02-373391	1
Fagron	Cloridrato de benzidamina	20E13-F02-373489	16
Fagron	Cloridrato de benzidamina	20E13-F02-373491	1
Fagron	Cloridrato de benzidamina	20K16-F04	1
Fagron	Cloridrato de benzidamina	2103302P	2
Fagron	Cloridrato de benzidamina	21G10-810-213932	2
Fagron	Cloridrato de benzidamina	21G10-B10	2
Fagron	Cloridrato de benzidamina	21G10-B10_213932	1
Fagron	Cloridrato de benzidamina	21G10-B10-2103932	1
Fagron	Cloridrato de benzidamina	21g10b10213932	1
Fagron	Cloridrato de benzidamina	21g10-b10-213932	1
Fagron	Cloridrato de benzidamina	21G10-B10-213932	22
Fagron	Cloridrato de benzidamina	21G10-B10-213932fagr	1
Fagron	Cloridrato de benzidamina	21G10-B10-219520	1
Fagron	Cloridrato de benzidamina	220830(21G10-B10-213932)	1
Fagron	Cloridrato de benzidamina	25021710	1
Fagron	Cloridrato de benzidamina	3280417	1
Fagron	Cloridrato de benzidamina	F02-3734809	5
Fargon/Noweda	Cloridrato de benzidamina	19K25-FO1-366695	1
Fargon	Cloridrato de benzidamina	21G10-B10-213932	1
Fragron	Cloridrato de benzidamina	18H29-B02-358711	1
Fresenius	Cloridrato de benzidamina	30062015099	1
Gehe	Cloridrato de benzidamina	18H29-B02-354329	1
Gehe	Cloridrato de benzidamina	21G10-B10-219520	1
Gehe	Cloridrato de benzidamina	AP300111801004B	1
GUMO	Cloridrato de benzidamina	19k25-f01	1
Noweda	Cloridrato de benzidamina	21G10-B10-219520	1
Phönix	Cloridrato de benzidamina	19K25-F01-366695	1
Phönix	Cloridrato de benzidamina	2003305P	1
Phönix	Cloridrato de benzidamina	f02-3734809	1
Sanacorp	Cloridrato de benzidamina	18H29-B02	1
SANACORP	Cloridrato de benzidamina	18H29-B02	1
Sanacorp	Cloridrato de benzidamina	18H29-Bo2-355663	1
Sanacorp	Cloridrato de benzidamina	20E13-F02-3734809	1
Sanacorp	Cloridrato de benzidamina	21G10-B10-213932	1

- 235 825 spectra from 1515 *Apo-Ident* customers from a total of 49 163 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de benzidamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de benzidamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	285	0	152 677
Type B	0	370	0	201 714
Type C	0	227	15	235 825

The substance/substance group *Cloridrato de benzidamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8947 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3784 %)
Type C	100.0000 % (> 99.9007 %)	93.8017 % (> 92.5620 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21699	21699	0,00	123,13
22268	21699	5,26	117,99
24411	25596	7,98	123,39
25596	25596	0,00	122,51
25718	21699	23,23	128,63
25781	25596	15,86	124,92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de bupivacaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24435-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de bupivacaína; Bupivacaína, cloridrato; Bupivacaini hydrochloridum

Special notes

When selecting the *Cloridrato de bupivacaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de bupivacaína	3	1	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de bupivacaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de bupivacaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	86,52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de bupivacaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de bupivacaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de bupivacaína	17E22-B08-345817	24435	40	1905513
Fagron	Cloridrato de bupivacaína	21J11-B06-219298	26464	40	20211202
Fagron	Cloridrato de bupivacaína	23A04-B09-233749	27026	40	20230209
Fagron	Cloridrato de bupivacaína	23A04-B09-233749	27026SI	20	20230209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *Cloridrato de bupivacaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 822 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Cloridrato de bupivacaína*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de bupivacaína	17L05-B04-358735	24594	40
Fagron	Cloridrato de bupivacaína	21J11-B06-219298	26464SI†	20

- 202 024 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de bupivacaína*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de bupivacaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de bupivacaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	55	5	202 024
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de bupivacaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9912 %)	91.6667 % (> 86.6667 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24435	24435	0,00	208,72
26464	24435	56,19	198,02
27026	24435	20,54	205,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de cetamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20278-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de cetamina; Cetamina, cloridrato; Ketamini hydrochloridum

Special notes

When selecting the *Cloridrato de cetamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de cetamina	6	5	88

Second-stage model

For differentiation of the substance/substance group *Cloridrato de cetamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de cetamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Omeprazol	115,04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de cetamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de cetamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de cetamina	2304005	26658	40	20230419*
Fagron	Cloridrato de cetamina	13H19-N01	21044	40	8931
Fagron	Cloridrato de cetamina	14I03-B02-303165	21779	60	20140926
Fagron	Cloridrato de cetamina	14I03-B02-311706	22533	40	20140926
Fagron	Cloridrato de cetamina	19H14-F02-364305	25295	40	20190918
Fagron	Cloridrato de cetamina	22F01-F01-385041	26909	40	20230727

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Cloridrato de cetamina*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Cloridrato de cetamina*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de cetamina	15E07-B03-322164	23201	40
Fagron	Cloridrato de cetamina	16E18-B03-339897	23941	40
Fagron	Cloridrato de cetamina	21D30-F02-378537	25759	40
Gatt-Koller	Cloridrato de cetamina	23J00824	26989	40
Gatt-Koller	Cloridrato de cetamina	23J01507	26990	40
Euro OTC	Cloridrato de cetamina	2304005	26658SI†	20
Fagron	Cloridrato de cetamina	21D30-F02-378537	25759SI	10
Fagron	Cloridrato de cetamina	22F01-F01-385041	26909SI†	40

- 201 814 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 261 spectra from 110 *Apo-Ident* customers from 97 batches from the substance/substance group *Cloridrato de cetamina*.
- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de cetamina	22F01-385047	1
	Cloridrato de cetamina	22F01-F01-385041	2
	Cloridrato de cetamina	2304005-01	5
	Cloridrato de cetamina	2304005-02	1
	Cloridrato de cetamina	2304005-03	5
	Cloridrato de cetamina	2304005-04	1
	Cloridrato de cetamina	2IL-13-F02-383873	1
AHD	Cloridrato de cetamina	2304005-02	1
Allergika Pharma / Phönix	Cloridrato de cetamina	21L13-F02-383872	1
Alliance Healthcare	Cloridrato de cetamina	21L13-F02-383872	1
Caelo	Cloridrato de cetamina	17K14-B01-355067	1
Caelo	Cloridrato de cetamina	21D30-F02-378863	1
Caesar & Loretz GmbH	Cloridrato de cetamina	700932-0001	1
Euro OTC	Cloridrato de cetamina	21D30-F02-378537	2
Euro OTC	Cloridrato de cetamina	21D3O-F02-378537	1
Euro OTC	Cloridrato de cetamina	2304005-01	1
Euro OTC	Cloridrato de cetamina	2304005-02	1
Euro OTC	Cloridrato de cetamina	F04-3734305	1
Fagron	Cloridrato de cetamina	/0321025	1
Fagron	Cloridrato de cetamina	14/03-B02-303165	1
Fagron	Cloridrato de cetamina	14/03-B02-309852	1
Fagron	Cloridrato de cetamina	14I03-B02-303165	1
Fagron	Cloridrato de cetamina	14I03-B02-309852	1
Fagron	Cloridrato de cetamina	15E07-B03-322164	5
Fagron	Cloridrato de cetamina	15E07-B03-327604	3
Fagron	Cloridrato de cetamina	16E18-B03	1
Fagron	Cloridrato de cetamina	16E18-B03-328264	2
Fagron	Cloridrato de cetamina	16E18-B03-330627	1
Fagron	Cloridrato de cetamina	16E18-B03-332957	3
Fagron	Cloridrato de cetamina	16E18-B03-334369	3
Fagron	Cloridrato de cetamina	16E18-B03-334370	1
Fagron	Cloridrato de cetamina	16E18-B03-335529	1
Fagron	Cloridrato de cetamina	16E18-B03-339897	4
Fagron	Cloridrato de cetamina	16E18-B03-339898	1
Fagron	Cloridrato de cetamina	16E18-B03-345971	2
Fagron	Cloridrato de cetamina	173017P	3
Fagron	Cloridrato de cetamina	17K14-B01-347995	4
Fagron	Cloridrato de cetamina	17K14-B01-347996	4
Fagron	Cloridrato de cetamina	17K14-B01-347997	1
Fagron	Cloridrato de cetamina	17K14-B01-3533344	1
Fagron	Cloridrato de cetamina	17K14B01353344	1
Fagron	Cloridrato de cetamina	17K14-B01-353344	1
Fagron	Cloridrato de cetamina	17K14-B01-356831	6
Fagron	Cloridrato de cetamina	17K14-B01-358396	8
Fagron	Cloridrato de cetamina	17K14-B01-358397	2
Fagron	Cloridrato de cetamina	182513P	1
Fagron	Cloridrato de cetamina	19H14-F02	6
Fagron	Cloridrato de cetamina	19h14-f02-364305	1
Fagron	Cloridrato de cetamina	19H14-F02-364305	9
Fagron	Cloridrato de cetamina	19H14-F02-364306	2
Fagron	Cloridrato de cetamina	19H14-F02-3650504	1
Fagron	Cloridrato de cetamina	19H14-F02365054	1
Fagron	Cloridrato de cetamina	19H14-F02-365054	5
Fagron	Cloridrato de cetamina	19H14-F07-3643005	1
Fagron	Cloridrato de cetamina	20A07-F01	2
Fagron	Cloridrato de cetamina	20a07-f01-368076	1
Fagron	Cloridrato de cetamina	20A07-F01368076	1
Fagron	Cloridrato de cetamina	20A07-F01-368076	8
Fagron	Cloridrato de cetamina	20A07-F01-368077	5
Fagron	Cloridrato de cetamina	20A07-F01-368078	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de cetamina	20A07-F01-3697602	1
Fagron	Cloridrato de cetamina	20A07-F01-369762	3
Fagron	Cloridrato de cetamina	20A07-F01-369763	3
Fagron	Cloridrato de cetamina	20G12-F04-373435	1
Fagron	Cloridrato de cetamina	20G13-F04	8
Fagron	Cloridrato de cetamina	20G13-F04-3729706	1
Fagron	Cloridrato de cetamina	20G13-F04-3729707	1
Fagron	Cloridrato de cetamina	20G13-F04-372976	1
Fagron	Cloridrato de cetamina	20G13-F04-372979	1
Fagron	Cloridrato de cetamina	20G13-F04-372981	1
Fagron	Cloridrato de cetamina	20G13-F04-373435	4
Fagron	Cloridrato de cetamina	21D033-F02-378538	1
Fagron	Cloridrato de cetamina	21D03-F02-378537	1
Fagron	Cloridrato de cetamina	21D30-F02	6
Fagron	Cloridrato de cetamina	21D30-F02-378537	6
Fagron	Cloridrato de cetamina	21D30-F02-378538	4
Fagron	Cloridrato de cetamina	21d30-F02-378863	1
Fagron	Cloridrato de cetamina	21D30-F02-378863	9
Fagron	Cloridrato de cetamina	21D30Fo2378537	1
Fagron	Cloridrato de cetamina	21D3OFO2378537	1
Fagron	Cloridrato de cetamina	21L13-F02	1
Fagron	Cloridrato de cetamina	21L13-F02-380925	13
Fagron	Cloridrato de cetamina	21L13-F02-381974	10
Fagron	Cloridrato de cetamina	21L13-F02-383872	4
Fagron	Cloridrato de cetamina	21L13-F02-383873	2
Fagron	Cloridrato de cetamina	21L13-FO2-381974	2
Fagron	Cloridrato de cetamina	F0136807006	1
Fagron	Cloridrato de cetamina	F01-3680707	1
Fagron	Cloridrato de cetamina	F02-3650504	1
Fagron	Cloridrato de cetamina	f02-3785307	1
Fagron	Cloridrato de cetamina	F02-3785307	1
Fagron	Cloridrato de cetamina	F02-3785308	1
Fagron	Cloridrato de cetamina	F04-3734305	3
Fagron	Cloridrato de cetamina	FO2-3788603	1
Fagron	Cloridrato de cetamina	SLL/KH/0321025	1
Fagron	Cloridrato de cetamina	SLL/KH/0422074	2
Fagron	Cloridrato de cetamina	SLL/KH/0520042	3
Fagron	Cloridrato de cetamina	SLL/KH/0719030	1
Fargon/Noweda	Cloridrato de cetamina	17K14-B01-356831	1
Fargron / Gehe	Cloridrato de cetamina	20G13-F04-373435	1
Gatt-Koller	Cloridrato de cetamina	1803056	1
GEHE 27.05.2014	Cloridrato de cetamina	13H19-N01	1
Gehe	Cloridrato de cetamina	19H14-F02-364305	1
Gehe	Cloridrato de cetamina	20A07-F01-368077	1
Gehe	Cloridrato de cetamina	20G13-F04-372976	1
Gehe	Cloridrato de cetamina	21D30-F02-378538	1
Gehe	Cloridrato de cetamina	22F01-F01-385041	2
jenne	Cloridrato de cetamina	2304005	1
Noweda	Cloridrato de cetamina	14/03-B02-311706	1
Noweda	Cloridrato de cetamina	292414P	1
Phoenix	Cloridrato de cetamina	F01-3680708	2
phönix	Cloridrato de cetamina	14103-B02-311706	1
Sanacorp	Cloridrato de cetamina	22F01-F01-385041	1

- 235 806 spectra from 1515 *Apo-Ident* customers from a total of 49 161 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de cetamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de cetamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	270	0	201 814
Type C	0	258	3	235 806

The substance/substance group *Cloridrato de cetamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	98.8506 % (> 97.7011 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21044	21044	0,00	133,89
21779	21044	15,04	138,29
22533	21044	8,56	133,35
25295	26658	10,73	131,93
26658	26658	0,00	128,86
26909	21044	57,51	114,20

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de ciprofloxacina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20945-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de ciprofloxacina; Ciprofloxacina, cloridrato; Ciprofloxacini hydrochloridum

Special notes

When selecting the *Cloridrato de ciprofloxacina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de ciprofloxacina	6	3	14

Second-stage model

For differentiation of the substance/substance group *Cloridrato de ciprofloxacina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de ciprofloxacina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	121,98	–
⋮	⋮	⋮
Cloridrato de quinina di-hidratado	>50	145,02
Citrato de sódio	>50	218,52
Metoxisaleno	>50	239,32
Capsaicina	>50	301,93
Piridoxal-5-fosfato	>50	321,92
Cloridrato de oxibutinina	>50	348,87
Prednicarbato	>50	384,07
Levocarnitina	>50	389,52
Heparina sódica	>50	409,69
Acetato de ciproterona	>50	473,69
Tetracaína	>50	673,99
Triclosan	>50	763,24
Cloridrato de amitriptilina	>50	960,51
Alfaestradiol	>50	1055,06
Acetato de noretisterona	>50	1193,48
Valina	>50	1303,32
Sacarose	>50	1402,14
Amifampridina	>50	1844,66

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de ciprofloxacina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de ciprofloxacina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de ciprofloxacina	12B08-N03	20945	40	1401421
Fagron	Cloridrato de ciprofloxacina	14B25-B02	21254	40	20140324

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de ciprofloxacina	16B17-B05-341882	23938	40	20160302
Fagron	Cloridrato de ciprofloxacina	18F27-B01-353346	24581	40	20180814
Fagron	Cloridrato de ciprofloxacina	20G01-F04-373719	25719	50	20200924
Fagron	Cloridrato de ciprofloxacina	21J08-B07-215636	26330	40	20220315
Fagron	Cloridrato de ciprofloxacina	21J08-B07-215636	26330SI	20	20220315

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Cloridrato de ciprofloxacina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 692 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Cloridrato de ciprofloxacina*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de ciprofloxacina	15D07-B01-312864	22755	40
Fagron	Cloridrato de ciprofloxacina	17K09-B02-345976	23991	40
Fagron	Cloridrato de ciprofloxacina	23F23-B08-228691	26898	40
Fagron	Cloridrato de ciprofloxacina	15D07-B01-312864	23568	40
Fagron	Cloridrato de ciprofloxacina	23F23-B08-228691	26898SI	20

- 201 904 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 12 *Apo-Ident* customers from 14 batches from the substance/substance group *Cloridrato de ciprofloxacina*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de ciprofloxacina	21J08-B07-223799	1
Caelo	Cloridrato de ciprofloxacina	16B17-B05-324218	1
Fagron	Cloridrato de ciprofloxacina	14/15-B08-303363	1
Fagron	Cloridrato de ciprofloxacina	14B25-B02-291783	2
Fagron	Cloridrato de ciprofloxacina	14B25-B02-291-783	1
Fagron	Cloridrato de ciprofloxacina	14F13-B01-303362	1
Fagron	Cloridrato de ciprofloxacina	14I15-B08	1
Fagron	Cloridrato de ciprofloxacina	14I15-B08-303363	1
Fagron	Cloridrato de ciprofloxacina	14l15-B08	1
Fagron	Cloridrato de ciprofloxacina	15D07-B01-312864	1
Fagron	Cloridrato de ciprofloxacina	17K09-B02-345976	1
Fagron	Cloridrato de ciprofloxacina	18F27-B01-363555	1
Fagron	Cloridrato de ciprofloxacina	CI0A003	1
Fargon/Anzag	Cloridrato de ciprofloxacina	F04-3737109	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de ciprofloxacina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de ciprofloxacina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	180	0	201 904
Type C	0	15	0	236 052

The substance/substance group *Cloridrato de ciprofloxacina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20945	20945	0,00	207,90
21254	20945	13,37	203,71
23938	20945	36,33	195,61
24581	20945	21,20	200,34
25719	20945	32,29	197,99
26330	20945	25,66	200,68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de cipro-heptadina 1,5-hidrato**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24437-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de cipro-heptadina 1,5-hidrato; Ciproeptadina, cloridrato hidratado; Cloridrato de ciproeptadina hidratado; Cyproheptadini hydrochloridum-1,5-hydricum

Special notes

When selecting the *Cloridrato de cipro-heptadina 1,5-hidrato* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de cipro-heptadina 1,5-hidrato	3	1	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	134,33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de cipro-hepta…	16K07-B01-350645	24437	40	1906179
Fagron	Cloridrato de cipro-hepta…	21H10-B06-219299	26634	40	20211207
Fagron	Cloridrato de cipro-hepta…	23G20-B01-231484	27027	40	20231025
Fagron	Cloridrato de cipro-hepta…	23G20-B01-231484	27027SI	20	20231025

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 822 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de cipro-hepta…	20K20-B05-202444	26076	40
Fagron	Cloridrato de cipro-hepta…	20K20-B05-202444	26076SI	20
Fagron	Cloridrato de cipro-hepta…	21H10-B06-219299	26634SI†	20

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato*

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

de cipro-heptadina 1,5-hidrato and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de cipro-heptadina 1,5-hidrato* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24437	24437	0,00	194,07
26634	24437	23,48	194,72
27027	24437	25,81	194,35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de cisteína monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20530-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de cisteína monoidratado; Cysteini hydrochloridum monohydricum

Special notes

When selecting the *Cloridrato de cisteína monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de cisteína monoidratado	9	4	4

Second-stage model

For differentiation of the substance/substance group *Cloridrato de cisteína monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de cisteína monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	102,76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de cisteína monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de cisteína monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de cisteína mo…	1701012	23003	40	20170207*
Euro OTC	Cloridrato de cisteína mo…	1706023	23548	40	20170721*
Euro OTC	Cloridrato de cisteína mo…	1807010-01	24188	40	20180808
Euro OTC	Cloridrato de cisteína mo…	1901012	24482	40	20190206*
Euro OTC	Cloridrato de cisteína mo…	2010020	25453	40	20201216*
Euro OTC	Cloridrato de cisteína mo…	2205018	26186	40	20220613*
Euro OTC	Cloridrato de cisteína mo…	2205018	26186SI	20	20220613*
Euro OTC	Cloridrato de cisteína mo…	2301029	26863	40	20230728*
Euro OTC	Cloridrato de cisteína mo…	2301029	26863SI	20	20230728*
Euro OTC	Cloridrato de cisteína mo…	2407009	27402	40	20241105*
Euro OTC	Cloridrato de cisteína mo…	2407009	27402SI	20	20241105*
Fagron	Cloridrato de cisteína mo…	22J13-B02	26447	40	20221207*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 12 reference samples from the substance/substance group *Cloridrato de cisteína monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 4 reference samples from the substance/substance group *Cloridrato de cisteína monoidratado*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de cisteína mo…	1304019-01	21325	40
Euro OTC	Cloridrato de cisteína mo…	1507006	21840	60
Euro OTC	Cloridrato de cisteína mo…	1510015	21941	60
Euro OTC	Cloridrato de cisteína mo…	1603018	22516	40

- 201 884 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Cloridrato de cisteína monoidratado*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de cisteína mo…	1304019-01	1
Euro OTC	Cloridrato de cisteína mo…	1807010-01	3
Euro OTC	Cloridrato de cisteína mo…	180710-01	1
Euro OTC	Cloridrato de cisteína mo…	1901012-01	1
Euro OTC	Cloridrato de cisteína mo…	2010020-01	2

- 236 059 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de cisteína monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de cisteína monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	200	0	201 884
Type C	0	8	0	236 059

The substance/substance group *Cloridrato de cisteína monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23003	23003	0,00	198,00
23548	23548	0,00	199,65

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24188	24482	7,82	197,97
24482	24482	0,00	201,91
25453	25453	0,00	196,71
26186	26186	0,00	198,65
26447	26447	0,00	205,64
26863	26863	0,00	202,24
27402	27402	0,00	205,98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de clindamicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20214-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de clindamicina; Clindamicina, cloridrato; Clindamycini hydrochloridum

Special notes

When selecting the *Cloridrato de clindamicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de clindamicina	11	13	324

Second-stage model

For differentiation of the substance/substance group *Cloridrato de clindamicina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de clindamicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	46,40	–
Sulfato de colistina	63,21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de clindamicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de clindamicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de clindamicina	15392809	22958	40	20151204
Caelo	Cloridrato de clindamicina	15392817	23245	40	20151204
Caelo	Cloridrato de clindamicina	21000113013	25927	40	20210212
Caelo	Cloridrato de clindamicina	21000113013	25927SI	40	20210212
Euro OTC	Cloridrato de clindamicina	1111058-01	20757	80	20120516
Euro OTC	Cloridrato de clindamicina	1511004	21996	60	20151123*
Euro OTC	Cloridrato de clindamicina	1510038	22224	60	20151120*
Euro OTC	Cloridrato de clindamicina	2001044	25074	40	20200303*
Euro OTC	Cloridrato de clindamicina	2004001	25307	40	20200804*
Euro OTC	Cloridrato de clindamicina	2004001	25307SI	40	20200804*
Fagron	Cloridrato de clindamicina	13G24-N09	21224	40	1412075
Fagron	Cloridrato de clindamicina	16D05-B08-332106	23264	40	20160504
Fagron	Cloridrato de clindamicina	24A23-B01-003404	27423	40	20240304
Fagron	Cloridrato de clindamicina	24A23-B01-003404	27423SI	40	20240304

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 640 spectra of 14 reference samples from the substance/substance group *Cloridrato de clindamicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 322 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 790 spectra of 20 reference samples from the substance/substance group *Cloridrato de clindamicina*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de clindamicina	153928	23365	40
Caelo	Cloridrato de clindamicina	172093	23681	40
Caelo	Cloridrato de clindamicina	22001232	26128	30
Caelo	Cloridrato de clindamicina	23003574	27135	40
Euro OTC	Cloridrato de clindamicina	1401041-01	21239	40
Euro OTC	Cloridrato de clindamicina	1710013	23769	40
Euro OTC	Cloridrato de clindamicina	1811003	24336	40
Euro OTC	Cloridrato de clindamicina	1903009	24637	40
Euro OTC	Cloridrato de clindamicina	2201043	25949	40
Euro OTC	Cloridrato de clindamicina	2208011	26341	40
Euro OTC	Cloridrato de clindamicina	2307031	26875	40
Euro OTC	Cloridrato de clindamicina	2410002	27452	40
Fagron	Cloridrato de clindamicina	23B24-B05-231501	26825	40
Caelo	Cloridrato de clindamicina	22001232	26128SI	40
Caelo	Cloridrato de clindamicina	23003574	27135SI	40
Euro OTC	Cloridrato de clindamicina	2201043	25949SI	40
Euro OTC	Cloridrato de clindamicina	2208011	26341SI	40
Euro OTC	Cloridrato de clindamicina	2307031	26875SI	40
Euro OTC	Cloridrato de clindamicina	2410002	27452SI	40
Fagron	Cloridrato de clindamicina	23B24-B05-231501	26825SI	40

- 201 294 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1085 spectra from 377 *Apo-Ident* customers from 336 batches from the substance/substance group *Cloridrato de clindamicina*.

- Among them are spectra of independent samples from 324 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de clindamicina	22001232004	2
	Cloridrato de clindamicina	22001232007	1
	Cloridrato de clindamicina	22001232008	7
	Cloridrato de clindamicina	22001232009	1
	Cloridrato de clindamicina	2208011-01	3
	Cloridrato de clindamicina	22A31-F04-383139	2
	Cloridrato de clindamicina	22A31-F04-382350	1
	Cloridrato de clindamicina	22G06-F01-383254	2
	Cloridrato de clindamicina	22G06-F01-383866	1
	Cloridrato de clindamicina	22G06-F01-383867	2
	Cloridrato de clindamicina	23003574001	2
	Cloridrato de clindamicina	23003574003	1
	Cloridrato de clindamicina	23B24-B05-235823	2
	Cloridrato de clindamicina	F0138325004	1
	Cloridrato de clindamicina	F01-3843600	2
	Cloridrato de clindamicina	F01-3843602	1
34543453	Cloridrato de clindamicina	5345435345	1
adfgafda	Cloridrato de clindamicina	dsgadgadfg	1
AHD	Cloridrato de clindamicina	130402X5	1
AHD	Cloridrato de clindamicina	16H03-B02-343063	1
AHD	Cloridrato de clindamicina	1710013-01	1
AHD	Cloridrato de clindamicina	23003574002	1
Anzag	Cloridrato de clindamicina	15392815	1
Bombastus	Cloridrato de clindamicina	1710013-01	1
Caelo	Cloridrato de clindamicina		1
Caelo	Cloridrato de clindamicina	10809406	1
Caelo	Cloridrato de clindamicina	1111058-03	1
Caelo	Cloridrato de clindamicina	11K04-N12	1
Caelo	Cloridrato de clindamicina	13G24-N09	1
Caelo	Cloridrato de clindamicina	1401041-01	2
Caelo	Cloridrato de clindamicina	140104102	1
Caelo	Cloridrato de clindamicina	14K04B05309851	1
Caelo	Cloridrato de clindamicina	151003801	2
Caelo	Cloridrato de clindamicina	1511004-01	3
Caelo	Cloridrato de clindamicina	1511004-02	1
Caelo	Cloridrato de clindamicina	1511004-03	2
Caelo	Cloridrato de clindamicina	15189512	1
Caelo	Cloridrato de clindamicina	15392802	1
Caelo	Cloridrato de clindamicina	15392804	4
Caelo	Cloridrato de clindamicina	15392805	1
Caelo	Cloridrato de clindamicina	15392807	1
Caelo	Cloridrato de clindamicina	15392811	2
Caelo	Cloridrato de clindamicina	15392814	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de clindamicina	15392815	4
Caelo	Cloridrato de clindamicina	15392816	1
Caelo	Cloridrato de clindamicina	15392817	3
Caelo	Cloridrato de clindamicina	15392818	2
Caelo	Cloridrato de clindamicina	15392819	1
Caelo	Cloridrato de clindamicina	15392822	2
Caelo	Cloridrato de clindamicina	15E06-B12-310472	1
Caelo	Cloridrato de clindamicina	15L22-B03-318788	1
Caelo	Cloridrato de clindamicina	160712C	2
Caelo	Cloridrato de clindamicina	16d05-b08-332106	1
Caelo	Cloridrato de clindamicina	16H03-B02	1
Caelo	Cloridrato de clindamicina	16H03-B02-336706	1
Caelo	Cloridrato de clindamicina	16H03-B02-339275	1
Caelo	Cloridrato de clindamicina	16H03-B03-334345	1
Caelo	Cloridrato de clindamicina	17001301	1
Caelo	Cloridrato de clindamicina	17209301	2
Caelo	Cloridrato de clindamicina	17209302	3
Caelo	Cloridrato de clindamicina	17209303	3
Caelo	Cloridrato de clindamicina	180009408	1
Caelo	Cloridrato de clindamicina	18009401	3
Caelo	Cloridrato de clindamicina	18009402	2
Caelo	Cloridrato de clindamicina	18009403	5
Caelo	Cloridrato de clindamicina	18009405	4
Caelo	Cloridrato de clindamicina	18009406	3
Caelo	Cloridrato de clindamicina	18009408	1
Caelo	Cloridrato de clindamicina	18009409	5
Caelo	Cloridrato de clindamicina	18009410	1
Caelo	Cloridrato de clindamicina	18009412	6
Caelo	Cloridrato de clindamicina	18009413	2
Caelo	Cloridrato de clindamicina	18009414	3
Caelo	Cloridrato de clindamicina	18009416	4
Caelo	Cloridrato de clindamicina	1811003-01	3
Caelo	Cloridrato de clindamicina	18A18-B08-346106	2
Caelo	Cloridrato de clindamicina	18A18-B08-346107	1
Caelo	Cloridrato de clindamicina	18D11-B01-349677	1
Caelo	Cloridrato de clindamicina	18J15-B04-355581	2
Caelo	Cloridrato de clindamicina	18J15-B04-358084	1
Caelo	Cloridrato de clindamicina	1903009-01	2
Caelo	Cloridrato de clindamicina	191332001	1
Caelo	Cloridrato de clindamicina	191392001	3
Caelo	Cloridrato de clindamicina	191392003	1
Caelo	Cloridrato de clindamicina	19139201	4
Caelo	Cloridrato de clindamicina	19139202	14
Caelo	Cloridrato de clindamicina	19139203	8
Caelo	Cloridrato de clindamicina	193087001	4
Caelo	Cloridrato de clindamicina	193087003	7
Caelo	Cloridrato de clindamicina	193087005	2
Caelo	Cloridrato de clindamicina	20001357001	3
Caelo	Cloridrato de clindamicina	20001357002	6
Caelo	Cloridrato de clindamicina	20001357003	3
Caelo	Cloridrato de clindamicina	20001357004	2
Caelo	Cloridrato de clindamicina	20001357005	7
Caelo	Cloridrato de clindamicina	20001357006	1
Caelo	Cloridrato de clindamicina	200035705	1
Caelo	Cloridrato de clindamicina	20004499001	3
Caelo	Cloridrato de clindamicina	20004499002	3
Caelo	Cloridrato de clindamicina	2072002	1
Caelo	Cloridrato de clindamicina	2100011300	1
Caelo	Cloridrato de clindamicina	21000113002	10
Caelo	Cloridrato de clindamicina	21000113003	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de clindamicina	21000113004	1
Caelo	Cloridrato de clindamicina	21000113005	1
Caelo	Cloridrato de clindamicina	21000113006	3
Caelo	Cloridrato de clindamicina	21000113007	8
Caelo	Cloridrato de clindamicina	21000113008	2
Caelo	Cloridrato de clindamicina	21000113009	1
Caelo	Cloridrato de clindamicina	21000113010	1
Caelo	Cloridrato de clindamicina	21000113011	2
Caelo	Cloridrato de clindamicina	21000113012	1
Caelo	Cloridrato de clindamicina	21000113013	8
Caelo	Cloridrato de clindamicina	21000113014	1
Caelo	Cloridrato de clindamicina	21000113015	1
Caelo	Cloridrato de clindamicina	2100113002	1
Caelo	Cloridrato de clindamicina	22001232002	1
Caelo	Cloridrato de clindamicina	22001232003	6
Caelo	Cloridrato de clindamicina	22001232008	1
Caelo	Cloridrato de clindamicina	3304	1
Caelo	Cloridrato de clindamicina	379/19AI	1
Caelo	Cloridrato de clindamicina	P-003-WS10100301	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	21000113005	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	19139202	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	19139203	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	21000113003	1
Caesar & Loretz GmbH/ E	Cloridrato de clindamicina	20004499002	1
Caesar & Loretz GmbH/Gehe	Cloridrato de clindamicina	193087003	1
Caesar & Loretz GmbH/Gehe	Cloridrato de clindamicina	22001232008	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	22001232004	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	20001357004	2
Caesar & Loretz GmbH...	Cloridrato de clindamicina	21000113004	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	F06-3643002	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	21000113004	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	21000113013	1
Caesar & Loretz GmbH...	Cloridrato de clindamicina	CN201810404	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	191392001	2
CAESAR & LORETZ GMBH	Cloridrato de clindamicina	191392001	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	19139201	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	19139202	4
Caesar & Loretz GmbH	Cloridrato de clindamicina	19139203	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	19190703	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	193087001	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	193087002	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	193087003	5
Caesar & Loretz GmbH	Cloridrato de clindamicina	193087004	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	19H28-F06-3643002	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	20001357001	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	20001357002	3
Caesar & Loretz GmbH	Cloridrato de clindamicina	20001357003	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	20001357004	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	20001357005	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	20004499001	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	20004499003	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113002	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113003	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113004	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113005	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113006	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113007	2
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113010	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113011	3
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113012	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de clindamicina	21000113015	3
Caesar & Loretz GmbH	Cloridrato de clindamicina	2100013015	1
Caesar & Loretz GmbH	Cloridrato de clindamicina	22001232002	6
Caesar & Loretz GmbH	Cloridrato de clindamicina	22001232003	6
Caesar & Loretz GmbH	Cloridrato de clindamicina	22001232004	3
Caesar & Loretz GmbH	Cloridrato de clindamicina	F06-3661407	1
Caesar & Loretz Hilden	Cloridrato de clindamicina	18009401	1
Cealo/AHD	Cloridrato de clindamicina	16D05-B08-325088	1
Cealo	Cloridrato de clindamicina	1111058-01	1
EuRho/Noweda	Cloridrato de clindamicina	2201043-01	1
EuRho	Cloridrato de clindamicina	1401041-01	1
EuRho	Cloridrato de clindamicina	1710013-01	1
Euro OTC	Cloridrato de clindamicina	1111058-01	6
Euro OTC	Cloridrato de clindamicina	1111058-02	2
Euro OTC	Cloridrato de clindamicina	1111058-03	3
Euro OTC	Cloridrato de clindamicina	111158-01	1
Euro OTC	Cloridrato de clindamicina	130709X8	2
Euro OTC	Cloridrato de clindamicina	140104101	1
Euro OTC	Cloridrato de clindamicina	1401041-01	11
Euro OTC	Cloridrato de clindamicina	140104102	3
Euro OTC	Cloridrato de clindamicina	1401041-02	6
Euro OTC	Cloridrato de clindamicina	1401401-01	1
Euro OTC	Cloridrato de clindamicina	150714B	1
Euro OTC	Cloridrato de clindamicina	150901B	1
Euro OTC	Cloridrato de clindamicina	1510030-01	1
Euro OTC	Cloridrato de clindamicina	151003502	1
Euro OTC	Cloridrato de clindamicina	1510038-01	20
Euro OTC	Cloridrato de clindamicina	1510038-02	4
Euro OTC	Cloridrato de clindamicina	1511004-002	1
Euro OTC	Cloridrato de clindamicina	151100401	2
Euro OTC	Cloridrato de clindamicina	1511004-01	15
Euro OTC	Cloridrato de clindamicina	1511004-02	4
Euro OTC	Cloridrato de clindamicina	1511004-03	2
Euro OTC	Cloridrato de clindamicina	16D05-B08-328259	1
Euro OTC	Cloridrato de clindamicina	16H03-B02-334974	1
Euro OTC	Cloridrato de clindamicina	16H03-B02-339275	1
Euro OTC	Cloridrato de clindamicina	171001301	2
Euro OTC	Cloridrato de clindamicina	1710013-01	29
Euro OTC	Cloridrato de clindamicina	1710019-01	1
Euro OTC	Cloridrato de clindamicina	1811003-01	13
Euro OTC	Cloridrato de clindamicina	1903009	1
Euro OTC	Cloridrato de clindamicina	1903009-01	31
Euro OTC	Cloridrato de clindamicina	200104401	1
Euro OTC	Cloridrato de clindamicina	2001044-01	21
Euro OTC	Cloridrato de clindamicina	200400101	2
Euro OTC	Cloridrato de clindamicina	2004001-01	18
Euro OTC	Cloridrato de clindamicina	2004001-02	1
Euro OTC	Cloridrato de clindamicina	2004001-03	1
Euro OTC	Cloridrato de clindamicina	2201043-01	13
Euro OTC	Cloridrato de clindamicina	220801-01	2
Euro OTC	Cloridrato de clindamicina	2208011-01	4
Euro OTC	Cloridrato de clindamicina	230703101	1
Euro OTC	Cloridrato de clindamicina	25071401	1
Euro OTC	Cloridrato de clindamicina	2908019-01	1
Euro OTC	Cloridrato de clindamicina	2908019V-03	4
Euro OTC	Cloridrato de clindamicina	4988149	1
Euro OTC	Cloridrato de clindamicina	700168	1
Euro OTC	Cloridrato de clindamicina	8061801	1
Euro OTC	Cloridrato de clindamicina	813M-03534	1
Euro OTC	Cloridrato de clindamicina	P-301-CN20181044	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de clindamicina	P-301-CN20210601	1
Euro OTC	Cloridrato de clindamicina	SCHE1107035	1
Euro OTC	Cloridrato de clindamicina	T03-05/1401041-01	1
Euro/Gehe16.03.16	Cloridrato de clindamicina	1510038-01	1
Europharm/Otto	Cloridrato de clindamicina	1111058-01	1
Fagron	Cloridrato de clindamicina	1010616	1
Fagron	Cloridrato de clindamicina	111105803	1
Fagron	Cloridrato de clindamicina	12C19-N06	1
Fagron	Cloridrato de clindamicina	12F19-N07	3
Fagron	Cloridrato de clindamicina	1370983	1
Fagron	Cloridrato de clindamicina	13A22/N01	1
Fagron	Cloridrato de clindamicina	13A22-N01	6
Fagron	Cloridrato de clindamicina	13C15-N06	1
Fagron	Cloridrato de clindamicina	13G24N09	1
Fagron	Cloridrato de clindamicina	13G24-N09	7
Fagron	Cloridrato de clindamicina	13J03-B02	1
Fagron	Cloridrato de clindamicina	13J03-B02_288654	1
Fagron	Cloridrato de clindamicina	13j03-B02-288653	1
Fagron	Cloridrato de clindamicina	13J03B02288654	1
Fagron	Cloridrato de clindamicina	13J03-B02-288654	3
Fagron	Cloridrato de clindamicina	13J03-B02-288655	1
Fagron	Cloridrato de clindamicina	14D23-B03	1
Fagron	Cloridrato de clindamicina	14K04-B05-304995	1
Fagron	Cloridrato de clindamicina	14K04-B05-304996	1
Fagron	Cloridrato de clindamicina	14K04-B05-309851	1
Fagron	Cloridrato de clindamicina	14K04-B05-313090	1
Fagron	Cloridrato de clindamicina	15E06-B12-310472	1
Fagron	Cloridrato de clindamicina	15E06-B12-311886	4
Fagron	Cloridrato de clindamicina	15E06-B12-313089	2
Fagron	Cloridrato de clindamicina	15E06-B12-314064	2
Fagron	Cloridrato de clindamicina	15E06-B12-314065	2
Fagron	Cloridrato de clindamicina	15E06-B12-314066	1
Fagron	Cloridrato de clindamicina	15L22-B03-316670	1
Fagron	Cloridrato de clindamicina	15L22-B03-318787	2
Fagron	Cloridrato de clindamicina	1600324C	1
Fagron	Cloridrato de clindamicina	160324C	2
Fagron	Cloridrato de clindamicina	16D05-B08	4
Fagron	Cloridrato de clindamicina	16D05-B08-320327	3
Fagron	Cloridrato de clindamicina	16D05-B08-321572	1
Fagron	Cloridrato de clindamicina	16D05-B08-323320	1
Fagron	Cloridrato de clindamicina	16D05-B08-323321	1
Fagron	Cloridrato de clindamicina	16D05-B08-325087	1
Fagron	Cloridrato de clindamicina	16D05-B08-325088	3
Fagron	Cloridrato de clindamicina	16d05-b08-325089	1
Fagron	Cloridrato de clindamicina	16D05B08327127	1
Fagron	Cloridrato de clindamicina	16D05-B08-327127	7
Fagron	Cloridrato de clindamicina	16D05-B08-328259	1
Fagron	Cloridrato de clindamicina	16D05-B08-328260	1
Fagron	Cloridrato de clindamicina	16D05-B08-330624	1
Fagron	Cloridrato de clindamicina	16D05-B08-332105	2
Fagron	Cloridrato de clindamicina	16D05-B08-332106	5
Fagron	Cloridrato de clindamicina	16d05-b08-332107	1
Fagron	Cloridrato de clindamicina	16D05-B08-332107	1
Fagron	Cloridrato de clindamicina	16H03-B02	5
Fagron	Cloridrato de clindamicina	16H03-B02-334344	2
Fagron	Cloridrato de clindamicina	16H03-B02-334345	1
Fagron	Cloridrato de clindamicina	16H03-B02-334974	1
Fagron	Cloridrato de clindamicina	16H03-B02-336706	5
Fagron	Cloridrato de clindamicina	16H03-B02-338802	2
Fagron	Cloridrato de clindamicina	16H03-B02-338803	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de clindamicina	16H03-B02-339275	1
Fagron	Cloridrato de clindamicina	16H03-B02-341602	2
Fagron	Cloridrato de clindamicina	16-H03-B02-341602	1
Fagron	Cloridrato de clindamicina	16H03-B02-39275	1
Fagron	Cloridrato de clindamicina	16HO3-B02-341602	1
Fagron	Cloridrato de clindamicina	17F22-B07-341603	1
Fagron	Cloridrato de clindamicina	18/15-B04-358084	2
Fagron	Cloridrato de clindamicina	18/15-B04-360142	1
Fagron	Cloridrato de clindamicina	18041801	1
Fagron	Cloridrato de clindamicina	1815B04355580	1
Fagron	Cloridrato de clindamicina	18A18-B08	4
Fagron	Cloridrato de clindamicina	18A18-B08-346106	1
Fagron	Cloridrato de clindamicina	18A18-B08-346107	2
Fagron	Cloridrato de clindamicina	18A18-B08-347483	7
Fagron	Cloridrato de clindamicina	18D11B01	1
Fagron	Cloridrato de clindamicina	18D11-B01	6
Fagron	Cloridrato de clindamicina	18D11-B01-349677	3
Fagron	Cloridrato de clindamicina	18D11-B01-351175	3
Fagron	Cloridrato de clindamicina	18D11-B01-351176	4
Fagron	Cloridrato de clindamicina	18D11-B01-351866	3
Fagron	Cloridrato de clindamicina	18D11-B01-352131	2
Fagron	Cloridrato de clindamicina	18D11-B01-352732	2
Fagron	Cloridrato de clindamicina	18D11-B01-352733	2
Fagron	Cloridrato de clindamicina	18D11-B01-353162	1
Fagron	Cloridrato de clindamicina	18J15-B04	4
Fagron	Cloridrato de clindamicina	18J15-B04-355579	4
Fagron	Cloridrato de clindamicina	18J15-B04-355580	1
Fagron	Cloridrato de clindamicina	18J15-b04-358082	1
Fagron	Cloridrato de clindamicina	18J15-B04-358082	1
Fagron	Cloridrato de clindamicina	18J15-B04-358084	1
Fagron	Cloridrato de clindamicina	18j15-b04-360142	1
Fagron	Cloridrato de clindamicina	18J15-B04-360142	8
Fagron	Cloridrato de clindamicina	18j15b04360143	1
Fagron	Cloridrato de clindamicina	19E23-B02-362301	1
Fagron	Cloridrato de clindamicina	19H28-F06	5
Fagron	Cloridrato de clindamicina	19H28-F06-364300	6
Fagron	Cloridrato de clindamicina	19H28-F06-3643000	1
Fagron	Cloridrato de clindamicina	19H28-F06-3643000855646	1
Fagron	Cloridrato de clindamicina	19H28-F06-364301	10
Fagron	Cloridrato de clindamicina	19H28-F06-364302	8
Fagron	Cloridrato de clindamicina	19H28-F06-366145	6
Fagron	Cloridrato de clindamicina	19H28-F06-366146	7
Fagron	Cloridrato de clindamicina	19H28-F06-366147	5
Fagron	Cloridrato de clindamicina	19H28-F06-366854	1
Fagron	Cloridrato de clindamicina	19H8-F06364302	1
Fagron	Cloridrato de clindamicina	20A27-F01	3
Fagron	Cloridrato de clindamicina	20A27-F01_369463	1
Fagron	Cloridrato de clindamicina	20A27-F01-3694602	1
Fagron	Cloridrato de clindamicina	20A27-F01-369462	2
Fagron	Cloridrato de clindamicina	20A27-F01-369463	7
Fagron	Cloridrato de clindamicina	20D07-F01	3
Fagron	Cloridrato de clindamicina	20D07-F01-370643	2
Fagron	Cloridrato de clindamicina	20D07-F01-370644	1
Fagron	Cloridrato de clindamicina	20D07-F01-370645	5
Fagron	Cloridrato de clindamicina	20D07-F01-370646	1
Fagron	Cloridrato de clindamicina	20D07F01-3709803	1
Fagron	Cloridrato de clindamicina	20D07-F01-370983	3
Fagron	Cloridrato de clindamicina	20H18-F02-374182	3
Fagron	Cloridrato de clindamicina	20J02F03376986	1
Fagron	Cloridrato de clindamicina	21D09-F01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de clindamicina	21D09-F01-3784605	1
Fagron	Cloridrato de clindamicina	21D09-F01-378464	1
Fagron	Cloridrato de clindamicina	21D09-F01-378465	6
Fagron	Cloridrato de clindamicina	21D09-F01-378495	1
Fagron	Cloridrato de clindamicina	21G01-F01	2
Fagron	Cloridrato de clindamicina	21G01-F01-379129	6
Fagron	Cloridrato de clindamicina	21G01-F01-379598	6
Fagron	Cloridrato de clindamicina	21G01F01379599	1
Fagron	Cloridrato de clindamicina	21G01-F01379599	1
Fagron	Cloridrato de clindamicina	21G01-F01-379599	12
Fagron	Cloridrato de clindamicina	21G01-F01-379600	10
Fagron	Cloridrato de clindamicina	2208011-01	1
Fagron	Cloridrato de clindamicina	22A31-F04-381645	2
Fagron	Cloridrato de clindamicina	22A31-F04-381646	2
Fagron	Cloridrato de clindamicina	22A31-F04-382349	1
Fagron	Cloridrato de clindamicina	22A31-F04-382350	2
Fagron	Cloridrato de clindamicina	22A31-F04-382351	3
Fagron	Cloridrato de clindamicina	22A31-F04-383139	2
Fagron	Cloridrato de clindamicina	2714Q-03534	1
Fagron	Cloridrato de clindamicina	2816	1
Fagron	Cloridrato de clindamicina	700168-0001	1
Fagron	Cloridrato de clindamicina	700168-0004	1
Fagron	Cloridrato de clindamicina	700168-0009	1
Fagron	Cloridrato de clindamicina	700168-F01-379600	1
Fagron	Cloridrato de clindamicina	B04-3580803	1
Fagron	Cloridrato de clindamicina	F01-3706404	1
Fagron	Cloridrato de clindamicina	F01-3706405	2
Fagron	Cloridrato de clindamicina	F01-370645	1
Fagron	Cloridrato de clindamicina	F01-3791209	1
Fagron	Cloridrato de clindamicina	F02-3741802	2
Fagron	Cloridrato de clindamicina	F03-3769806	1
Fagron	Cloridrato de clindamicina	F06-3643000	1
Fagron	Cloridrato de clindamicina	F06-3643002	1
Fagron	Cloridrato de clindamicina	F06-3661405	1
Fagron	Cloridrato de clindamicina	Fagron20H18-F02-374182	1
Fagron	Cloridrato de clindamicina	K-171217B	2
Fagron	Cloridrato de clindamicina	K-171219B	2
Fagron	Cloridrato de clindamicina	K-180507B	8
Fagron	Cloridrato de clindamicina	K-190507B	1
Fagron	Cloridrato de clindamicina	K-190610B	7
Fagron	Cloridrato de clindamicina	K-190909B	1
Fagron	Cloridrato de clindamicina	K-191226B	1
Fagron	Cloridrato de clindamicina	K-200516B	1
Fagron	Cloridrato de clindamicina	k-210407B	1
Fagron	Cloridrato de clindamicina	K-210407B	4
Fagron	Cloridrato de clindamicina	P-003-CN20150406	1
Fagron	Cloridrato de clindamicina	P003-WS10100301	1
Fagron	Cloridrato de clindamicina	P003WS13091401	1
Fagrun	Cloridrato de clindamicina	18A18-B08-346107	1
Fargon/Noweda	Cloridrato de clindamicina	18D11-B01	1
Fargon/Sanacorp	Cloridrato de clindamicina	K-180507B	1
Fargon	Cloridrato de clindamicina	11L20-No5	1
Fargon	Cloridrato de clindamicina	16D05-B08-320327	1
Fargron/Noweda	Cloridrato de clindamicina	18J15-B04-358084	1
Fargron/Noweda	Cloridrato de clindamicina	19H28-F06-364302	3
Fiebig	Cloridrato de clindamicina	11023741802	1
Fiebig	Cloridrato de clindamicina	f01-3706405	1
Fiebig	Cloridrato de clindamicina	F06-3643002	1
Fiebig	Cloridrato de clindamicina	K-190909B	1
Gehe/ Euro	Cloridrato de clindamicina	1903009-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe/EuRho	Cloridrato de clindamicina	2004001-01	1
Gehe/EuRho	Cloridrato de clindamicina	2208011-01	1
Gehe	Cloridrato de clindamicina	11E12-N02	1
Gehe	Cloridrato de clindamicina	11K04-N12	1
Gehe	Cloridrato de clindamicina	13a22-n01	1
Gehe	Cloridrato de clindamicina	13A22-N01	1
GEHE	Cloridrato de clindamicina	1811003-01	1
Gehe	Cloridrato de clindamicina	19H28-F06	1
Gehe	Cloridrato de clindamicina	20A27-F01-369462	1
Gehe	Cloridrato de clindamicina	22G06-F01-383866	1
Gehe	Cloridrato de clindamicina	22G06-F01-383867	1
Gehe	Cloridrato de clindamicina	700168-0002	1
Gehe	Cloridrato de clindamicina	K-210407B	1
gfsdgs	Cloridrato de clindamicina	sgfsgf	1
GUMO	Cloridrato de clindamicina	21000113010	1
hfdhsdhsh	Cloridrato de clindamicina	dfhdhsd	1
Jenne	Cloridrato de clindamicina	18D11-B01-352732	2
Jenne	Cloridrato de clindamicina	18J15-B04-360142	1
L12	Cloridrato de clindamicina	17209302	1
L12	Cloridrato de clindamicina	18009402	2
L12	Cloridrato de clindamicina	18009403	2
L30	Cloridrato de clindamicina	17209301	1
Noweda/EuRho	Cloridrato de clindamicina	2201043-01	1
noweda	Cloridrato de clindamicina	1511004-03	1
Noweda	Cloridrato de clindamicina	1811003-01	1
Noweda	Cloridrato de clindamicina	18D11-B01-351176	1
Noweda	Cloridrato de clindamicina	22001232002	1
Noweda	Cloridrato de clindamicina	22001232003	2
Noweda	Cloridrato de clindamicina	22G06-F01	1
Noweda	Cloridrato de clindamicina	22G06-F01-383867	1
Noweda	Cloridrato de clindamicina	2908019V-03	1
Otto Geilenkirchen	Cloridrato de clindamicina	200400101	1
Phoenix 5.12.2018	Cloridrato de clindamicina	18A18-B08-346106	1
Phoenix	Cloridrato de clindamicina	16D05-B08-327127	1
Phoenix	Cloridrato de clindamicina	1710013-010	1
Phoenix	Cloridrato de clindamicina	1811003-01	1
Phoenix	Cloridrato de clindamicina	2004001-01	1
Phoenix	Cloridrato de clindamicina	3367	1
Phoenix	Cloridrato de clindamicina	K-171217B	1
Phönix	Cloridrato de clindamicina	12H30-N04	1
Phönix	Cloridrato de clindamicina	15392803	1
phönix	Cloridrato de clindamicina	15392820	1
Phönix	Cloridrato de clindamicina	193087005	1
Phönix	Cloridrato de clindamicina	2001044-01	1
Phönix	Cloridrato de clindamicina	20D07-F011	1
rfgrgrgr	Cloridrato de clindamicina		1
Sanacorp	Cloridrato de clindamicina	1511004-03	1
Sanacorp	Cloridrato de clindamicina	16D05-B08-332106	1
Sanacorp	Cloridrato de clindamicina	16H03-B02-339275	1
Sanacorp	Cloridrato de clindamicina	16H03-B02-341602	1
Sanacorp	Cloridrato de clindamicina	18A18-B08-347483	1
Sanacorp	Cloridrato de clindamicina	18D11-B01-352732	1
Sanacorp	Cloridrato de clindamicina	21462-39-S	1
Sanacorp	Cloridrato de clindamicina	21G01-F01-379600	1
Sanacorp	Cloridrato de clindamicina	220801-01	1
Sanacorp	Cloridrato de clindamicina	2208011-01	1
Sanacorp	Cloridrato de clindamicina	22G06-F01-384360	2
Sanacorp	Cloridrato de clindamicina	F01-3694602	1
Sanacorp	Cloridrato de clindamicina	K-171219B	1
Sanacorp	Cloridrato de clindamicina	K-180507B	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spangro 22.05.2014	Cloridrato de clindamicina	13G24-N09	1
Spangro_04.04.2019	Cloridrato de clindamicina	18D11-B01-352131	1

- 234 982 spectra from 1515 *Apo-Ident* customers from a total of 48 925 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de clindamicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de clindamicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	640	0	152 322
Type B	0	790	0	201 294
Type C	0	1078	7	234 982

The substance/substance group *Cloridrato de clindamicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0625 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2405 %)
Type C	100.0000 % (> 99.9007 %)	99.3548 % (> 99.0783 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20757	21996	8,10	70,47
21224	21224	0,00	71,79
21996	21996	0,00	70,72
22224	22224	0,00	69,82

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22958	22224	9,12	71,11
23245	22224	3,74	70,19
23264	21996	3,44	70,07
25074	25074	0,00	69,59
25307	25307	0,00	71,97
25927	21996	13,84	69,65
27423	21996	18,82	72,68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de clonidina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20637-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de clonidina; Clonidina, cloridrato; Clonidini hydrochloridum

Special notes

When selecting the *Cloridrato de clonidina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de clonidina	6	4	11

Second-stage model

For differentiation of the substance/substance group *Cloridrato de clonidina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de clonidina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	123,39	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de clonidina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de clonidina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de clonidina	13I25-B07	21220	40	20131009
Fagron	Cloridrato de clonidina	14H11-B04-311163	21966	60	AR-18-FG-006797-02
Fagron	Cloridrato de clonidina	14H11-B04-311163	22967	40	20140929
Fagron	Cloridrato de clonidina	14H11-B04-311163	22967SI	40	20140929
Fagron	Cloridrato de clonidina	19B27-B02-361777	24687	40	20190607
Fagron	Cloridrato de clonidina	22A26-B04-216708	26141	40	20220316
Fagron	Cloridrato de clonidina	22A26-B04-216708	26141SI	40	20220316
Fagron	Cloridrato de clonidina	22B22-B03-216999	26142	40	20220505
Fagron	Cloridrato de clonidina	22B22-B03-216999	26142SI	40	20220505
Fagron	Cloridrato de clonidina	24A29-B05-234630	27186	40	20240227

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Cloridrato de clonidina*. These samples are listed above in the *calibration samples* section. The reference samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

come from 6 different batches.

- 152 542 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 13 reference samples from the substance/substance group *Cloridrato de clonidina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de clonidina	15L11-B01-332270	23228	40
Fagron	Cloridrato de clonidina	18B12-B04-353341	24443	40
Fagron	Cloridrato de clonidina	20D29-F02-374142	25785	40
Fagron	Cloridrato de clonidina	21F07-B03-213617	25907	40
Fagron	Cloridrato de clonidina	14H11-B04-311163	21966SI†	60
Fagron	Cloridrato de clonidina	15L11-B01-332270	23228SI	40
Fagron	Cloridrato de clonidina	15L11-B01-332270	23410	40
Fagron	Cloridrato de clonidina	15L11-B01-332270	23410SI	40
Fagron	Cloridrato de clonidina	18B12-B04-353341	24443SI	40
Fagron	Cloridrato de clonidina	19B27-B02-361777	24687SI†	40
Fagron	Cloridrato de clonidina	20D29-F02-374142	25785SI	40
Fagron	Cloridrato de clonidina	21F07-B03-213617	25907SI	40
Fagron	Cloridrato de clonidina	24A29-B05-234630	27186SI†	40

- 201 544 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 56 spectra from 18 *Apo-Ident* customers from 12 batches from the substance/substance group *Cloridrato de clonidina*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de clonidina	22B22-B03-225373	1
Fagron	Cloridrato de clonidina	14H11-B04-298642	1
Fagron	Cloridrato de clonidina	14H11-B04-311163	42
Fagron	Cloridrato de clonidina	15L11-B01	1
Fagron	Cloridrato de clonidina	18B12-B04-353341	1
Fagron	Cloridrato de clonidina	20D29-F02-3705608	1
Fagron	Cloridrato de clonidina	20D29-F02-370567	1
Fagron	Cloridrato de clonidina	21F07-B03-213617	1
Fagron	Cloridrato de clonidina	22B22-B03-217792	1
Fagron	Cloridrato de clonidina	22B22-B03-221078	2
Fagron	Cloridrato de clonidina	22B22-B03-225373	1
Fagron	Cloridrato de clonidina	77543E004	1
Fagron	Cloridrato de clonidina	F02-370567	1
Regenbogen Apotheke	Cloridrato de clonidina	18B12-B04-353341	1

- 236 011 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de clonidina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de clonidina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	540	0	201 544
Type C	0	56	0	236 011

The substance/substance group *Cloridrato de clonidina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 89.2857 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21220	21966	21,49	209,07
21966	21966	0,00	230,46
22967	21966	29,57	206,71
24687	21966	34,96	207,22
26141	21966	32,84	207,07
26142	21966	40,04	208,88
27186	21966	47,04	209,34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de cloreto de tiamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20566-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de cloreto de tiamina; Tiamina, cloridrato de cloreto

Special notes

When selecting the *Cloridrato de cloreto de tiamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de cloreto de tiamina	9	11	38

Second-stage model

For differentiation of the substance/substance group *Cloridrato de cloreto de tiamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de cloreto de tiamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	88,79	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de cloreto de tiamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de cloreto de tiamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de cloreto de …	14069502	21478	60	20140321
Caelo	Cloridrato de cloreto de …	14069502	21511	60	8986
Caelo	Cloridrato de cloreto de …	160156	22477	60	20160316*
Caelo	Cloridrato de cloreto de …	192567	25095	40	20191216*
Caelo	Cloridrato de cloreto de …	20001173	25193	40	20200724*
Euro OTC	Cloridrato de cloreto de …	1211008-02	21647	60	20121122
Euro OTC	Cloridrato de cloreto de …	1612004	22919	40	20170117*
Euro OTC	Cloridrato de cloreto de …	2004007	25274	40	20200618*
Euro OTC	Cloridrato de cloreto de …	2007034	25332	40	20200909*
Euro OTC	Cloridrato de cloreto de …	2309008	26928	40	20231006*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 10 reference samples from the substance/substance group *Cloridrato de cloreto de tiamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 482 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 475 spectra of 14 reference samples from the substance/substance group *Cloridrato de cloreto de tiamina*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de cloreto de …	170976	23368	40
Caelo	Cloridrato de cloreto de …	21002868002	26416	30
Caelo	Cloridrato de cloreto de …	22003533	26482	40
Caelo	Cloridrato de cloreto de …	23001172	26835	40
Euro OTC	Cloridrato de cloreto de …	1705034	23439	40
Euro OTC	Cloridrato de cloreto de …	1712013	23911	40
Euro OTC	Cloridrato de cloreto de …	1807001	24146	40
Euro OTC	Cloridrato de cloreto de …	2201045	25961	40
Euro OTC	Cloridrato de cloreto de …	2207008	26211	40
Fagron	Cloridrato de cloreto de …	22I22-B05-223757	26536	40
Fagron	Cloridrato de cloreto de …	23G04-B12-239937	27191	40
Caelo	Cloridrato de cloreto de …	22003533	26482SI	20
Euro OTC	Cloridrato de cloreto de …	2201045	25961SI	5
Euro OTC	Cloridrato de cloreto de …	2207008	26211SI	20

- 201 609 spectra from a total of 4034 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 62 spectra from 28 *Apo-Ident* customers from 40 batches from the substance/substance group *Cloridrato de cloreto de tiamina*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de cloreto de ...		1
Caelo	Cloridrato de cloreto de ...	11061401	1
Caelo	Cloridrato de cloreto de ...	11371309	2
Caelo	Cloridrato de cloreto de ...	11371313	1
Caelo	Cloridrato de cloreto de ...	11371319	3
Caelo	Cloridrato de cloreto de ...	12091407	1
Caelo	Cloridrato de cloreto de ...	12340712	1
Caelo	Cloridrato de cloreto de ...	13296610	4
Caelo	Cloridrato de cloreto de ...	14069502	1
Caelo	Cloridrato de cloreto de ...	15003201	1
Caelo	Cloridrato de cloreto de ...	15199009	2
Caelo	Cloridrato de cloreto de ...	15199099	1
Caelo	Cloridrato de cloreto de ...	15269613	1
Caelo	Cloridrato de cloreto de ...	16015607	1
Caelo	Cloridrato de cloreto de ...	16015609	1
Caelo	Cloridrato de cloreto de ...	17097602	1
Caelo	Cloridrato de cloreto de ...	171201301	1
Caelo	Cloridrato de cloreto de ...	18163717	2
Caelo	Cloridrato de cloreto de ...	20001173002	2
Caelo	Cloridrato de cloreto de ...	20004527005	1
Caelo	Cloridrato de cloreto de ...	4071402	1
Caelo	Cloridrato de cloreto de ...	5122	1
Caelo	Cloridrato de cloreto de ...	8121405	1
Caesar & Loretz GmbH	Cloridrato de cloreto de ...	18163705	1
Caesar & Loretz GmbH	Cloridrato de cloreto de ...	18163709	2
Caesar & Loretz GmbH	Cloridrato de cloreto de ...	18163717	1
Caesar & Loretz GmbH	Cloridrato de cloreto de ...	20004527005	5
Euro OTC	Cloridrato de cloreto de ...	1211008-01	1
Euro OTC	Cloridrato de cloreto de ...	161200401	1
Euro OTC	Cloridrato de cloreto de ...	1705034-01	2
Euro OTC	Cloridrato de cloreto de ...	1712013-01	1
Euro OTC	Cloridrato de cloreto de ...	1807001-01	3
Euro OTC	Cloridrato de cloreto de ...	2004007-01	1
Euro OTC	Cloridrato de cloreto de ...	2007034-01	1
Euro OTC	Cloridrato de cloreto de ...	2207008-01	1
Fagron	Cloridrato de cloreto de ...	10111401	1
Fagron	Cloridrato de cloreto de ...	13E22-No8	1
Fagron	Cloridrato de cloreto de ...	17F23-B02-340810	1
Fagron	Cloridrato de cloreto de ...	190115006	1
Fagron	Cloridrato de cloreto de ...	20A13-B08-196821	1
Fagron	Cloridrato de cloreto de ...	20F16-B09-201351	2
Finze	Cloridrato de cloreto de ...	9216114	1
Jiangxi Tianxin	Cloridrato de cloreto de ...	1807001-01	1
Sanacorp	Cloridrato de cloreto de ...	12340712	1

- 236 005 spectra from 1515 *Apo-Ident* customers from a total of 49 219 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de cloreto de tiamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de cloreto de tiamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	475	0	201 609
Type C	0	62	0	236 005

The substance/substance group *Cloridrato de cloreto de tiamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7368 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.3226 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21478	25274	11,78	173,85
21511	21511	0,00	181,83
21647	22477	10,49	191,24
22477	22477	0,00	201,46
22919	22919	0,00	181,19
25095	25095	0,00	180,33
25193	25193	0,00	186,43
25274	25274	0,00	177,26
25332	25332	0,00	169,43
26928	26928	0,00	159,81

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de clorprotixeno**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24105-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de clorprotixeno; Chlorprothixeni hydrochloridum; Clorprotixeno, cloridrato

Special notes

When selecting the *Cloridrato de clorprotixeno* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de clorprotixeno	2	1	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de clorprotixeno* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de clorprotixeno* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de doxepina	35,76	–
Cloridrato de benzidamina	131,27	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de clorprotixeno* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de clorprotixeno*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Cloridrato de clorprotixeno	AP05061117C	24105	40	1810394
Euro OTC	Cloridrato de clorprotixeno	2003005	25290	40	20200728*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Cloridrato de clorprotixeno*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Cloridrato de clorprotixeno*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Cloridrato de clorprotixeno	AP04120418C	24434	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de clorprotixeno*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de clorprotixeno* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de clorprotixeno* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect.

The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de clorprotixeno* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24105	24105	0,00	61,52
25290	25290	0,00	62,24

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de clortetraciclina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20845-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de clortetraciclina; Chlortetracyclini hydrochloridum; Clortetraciclina, cloridrato

Special notes

When selecting the *Cloridrato de clortetraciclina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de clortetraciclina	7	4	90

Second-stage model

For differentiation of the substance/substance group *Cloridrato de clortetraciclina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de clortetraciclina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de tetraciclina	57,52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de clortetraciclina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de clortetraciclina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de clortetraciclina	1108051-02	21241	40	20111013
Euro OTC	Cloridrato de clortetraciclina	1604015	22541	40	20160510*
Euro OTC	Cloridrato de clortetraciclina	1910002	24959	40	20191107*
Euro OTC	Cloridrato de clortetraciclina	2009026	25573	40	20210104*
Euro OTC	Cloridrato de clortetraciclina	2205011	26229	40	20220704*
Fagron	Cloridrato de clortetraciclina	12K30-N07	20845	40	1405318
Fagron	Cloridrato de clortetraciclina	12K30-N07	21222	40	20121210
Fagron	Cloridrato de clortetraciclina	14J08-B07-307742	21877	60	20141029

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 340 spectra of 8 reference samples from the substance/substance group *Cloridrato de clortetraciclina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Cloridrato de clortetraciclina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de clortetraciclina	1604015-01	22975	40
Euro OTC	Cloridrato de clortetraciclina	1803037	24092	40
Euro OTC	Cloridrato de clortetraciclina	2402024	27365	40
Fagron	Cloridrato de clortetraciclina	16B10-B09-329778	23571	30
Euro OTC	Cloridrato de clortetraciclina	2205011	26229SI†	20
Euro OTC	Cloridrato de clortetraciclina	2402024	27365SI	20

- 201 894 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 673 spectra from 302 *Apo-Ident* customers from 102 batches from the substance/substance group *Cloridrato de clortetraciclina*.

- Among them are spectra of independent samples from 89 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de clortetraciclina	2009026-01	2
	Cloridrato de clortetraciclina	2205011-01	5
AHD/Euro	Cloridrato de clortetraciclina	1803037	2
ALH	Cloridrato de clortetraciclina	16B10-B09-320304	1
Alliance Healthcare	Cloridrato de clortetraciclina	12K30-N07	1
Anzag/ Euro OT	Cloridrato de clortetraciclina	1803037-02	1
Anzag: 07.09.12 ek:4.01	Cloridrato de clortetraciclina	12C16-N01	1
Anzag	Cloridrato de clortetraciclina	1604015-01	1
apo-ident	Cloridrato de clortetraciclina	1803037-01	2
apomix	Cloridrato de clortetraciclina	2009026-01	1
Caelo	Cloridrato de clortetraciclina		1
Caelo	Cloridrato de clortetraciclina	1108051-01	2
Caelo	Cloridrato de clortetraciclina	1412008-01	1
Caelo	Cloridrato de clortetraciclina	141200802	1
Caelo	Cloridrato de clortetraciclina	1412008-02	1
Caelo	Cloridrato de clortetraciclina	141200803	1
Caelo	Cloridrato de clortetraciclina	142008-03	1
Caelo	Cloridrato de clortetraciclina	14J08-B07-300249	1
Caelo	Cloridrato de clortetraciclina	14J08-B07-303352	1
Caelo	Cloridrato de clortetraciclina	14j08-b07-307100	1
Caelo	Cloridrato de clortetraciclina	1604015-01	4
Caelo	Cloridrato de clortetraciclina	1604015-61	1
Caelo	Cloridrato de clortetraciclina	16B10-B09-318088	1
Caelo	Cloridrato de clortetraciclina	16B10-B09-322716	1
Caelo	Cloridrato de clortetraciclina	16B10B09329778	1
Caelo	Cloridrato de clortetraciclina	16B10-B09-336332	1
Caelo	Cloridrato de clortetraciclina	16B10-B09-347439	3
Caelo	Cloridrato de clortetraciclina	1803037-01	3
Caelo	Cloridrato de clortetraciclina	1803037-03	1
Caelo	Cloridrato de clortetraciclina	1803038-01	1
Caelo	Cloridrato de clortetraciclina	1910002-01	1
Caelo	Cloridrato de clortetraciclina	191002-02	1
Caelo	Cloridrato de clortetraciclina	FC13030134	1
Caelo	Cloridrato de clortetraciclina	FC15100204	1
Caesar & Loretz GmbH	Cloridrato de clortetraciclina	12C16-N01	1
EuRho/ AHD	Cloridrato de clortetraciclina	1803037-01	5
EuRho/ NOWEDA	Cloridrato de clortetraciclina	1803037-02	1
Eurho/Fiebig	Cloridrato de clortetraciclina	1910002-01	1
EuRho/Gehe	Cloridrato de clortetraciclina	1803037	1
EuRho/Gehe	Cloridrato de clortetraciclina	2009026-01	1
Eurho/Phönix	Cloridrato de clortetraciclina	220501101	1
EuRho	Cloridrato de clortetraciclina	1412008-02	1
EuRho	Cloridrato de clortetraciclina	1803037-01	1
EuRho	Cloridrato de clortetraciclina	1910002-01	2
Euro OTC	Cloridrato de clortetraciclina		1
Euro OTC	Cloridrato de clortetraciclina	10I29-N04	1
Euro OTC	Cloridrato de clortetraciclina	1108051-01	6
Euro OTC	Cloridrato de clortetraciclina	110805102	1
Euro OTC	Cloridrato de clortetraciclina	1108051-02	7
Euro OTC	Cloridrato de clortetraciclina	1412008/03	1
Euro OTC	Cloridrato de clortetraciclina	1412008-01	9
Euro OTC	Cloridrato de clortetraciclina	141200802	2
Euro OTC	Cloridrato de clortetraciclina	1412008-02	15
Euro OTC	Cloridrato de clortetraciclina	141200803	1
Euro OTC	Cloridrato de clortetraciclina	1412008-03	5
Euro OTC	Cloridrato de clortetraciclina	16004015-15	1
Euro OTC	Cloridrato de clortetraciclina	160401501	2
Euro OTC	Cloridrato de clortetraciclina	1604015-01	61
Euro OTC	Cloridrato de clortetraciclina	160401502	1
Euro OTC	Cloridrato de clortetraciclina	1604015-02	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de clortetraciclina	16b10-b09-326865	1
Euro OTC	Cloridrato de clortetraciclina	16B10-B09-348359	1
Euro OTC	Cloridrato de clortetraciclina	16B10-B09-352970	1
Euro OTC	Cloridrato de clortetraciclina	1803037	2
Euro OTC	Cloridrato de clortetraciclina	1803037_01	4
Euro OTC	Cloridrato de clortetraciclina	180303701	1
Euro OTC	Cloridrato de clortetraciclina	1803037-01	61
Euro OTC	Cloridrato de clortetraciclina	1803037-02	3
Euro OTC	Cloridrato de clortetraciclina	1803037-03	22
Euro OTC	Cloridrato de clortetraciclina	190002-02	1
Euro OTC	Cloridrato de clortetraciclina	19100002-02	1
Euro OTC	Cloridrato de clortetraciclina	1910002	1
Euro OTC	Cloridrato de clortetraciclina	191000201	1
Euro OTC	Cloridrato de clortetraciclina	1910002-01	85
Euro OTC	Cloridrato de clortetraciclina	1910002-02	26
Euro OTC	Cloridrato de clortetraciclina	191002-01	2
Euro OTC	Cloridrato de clortetraciclina	200902601	1
Euro OTC	Cloridrato de clortetraciclina	2009026-01	59
Euro OTC	Cloridrato de clortetraciclina	2009026-02	2
Euro OTC	Cloridrato de clortetraciclina	2205011-01	1
Euro OTC	Cloridrato de clortetraciclina	2901009V-03	1
Euro OTC	Cloridrato de clortetraciclina	4612Q-01155	1
Euro OTC	Cloridrato de clortetraciclina	4931439	1
Euro OTC	Cloridrato de clortetraciclina	5113I01155	1
Euro OTC	Cloridrato de clortetraciclina	700156	1
Euro OTC	Cloridrato de clortetraciclina	80218-A	1
Euro OTC	Cloridrato de clortetraciclina	FC15110253	1
Euro OTC	Cloridrato de clortetraciclina	FC21020106	1
EURO Pharma	Cloridrato de clortetraciclina	1108051-01	1
EUro/AHD	Cloridrato de clortetraciclina	1108051-02	1
euro/gehe	Cloridrato de clortetraciclina	1604015-01	1
Euro/Noweda	Cloridrato de clortetraciclina	1604015-01	1
EuRo/Phönix	Cloridrato de clortetraciclina	160401501	1
Euro/Phönix	Cloridrato de clortetraciclina	2009026-01	2
Euro	Cloridrato de clortetraciclina	1108051-02	1
Fagron	Cloridrato de clortetraciclina		1
Fagron	Cloridrato de clortetraciclina	12C16-N01	1
Fagron	Cloridrato de clortetraciclina	12H28N09	1
Fagron	Cloridrato de clortetraciclina	12H28-N09	4
Fagron	Cloridrato de clortetraciclina	12k30-N07	1
Fagron	Cloridrato de clortetraciclina	12K30-N07	9
Fagron	Cloridrato de clortetraciclina	13/11-N07	4
Fagron	Cloridrato de clortetraciclina	13K26-N06	2
Fagron	Cloridrato de clortetraciclina	13l11-N07	1
Fagron	Cloridrato de clortetraciclina	14J08-B07	4
Fagron	Cloridrato de clortetraciclina	14J08-B07-300247	2
Fagron	Cloridrato de clortetraciclina	14J08-B07-300250	8
Fagron	Cloridrato de clortetraciclina	14J08-B07-303350	1
Fagron	Cloridrato de clortetraciclina	14J08-B07-303352	7
Fagron	Cloridrato de clortetraciclina	14J08B07307100	3
Fagron	Cloridrato de clortetraciclina	14J08-B07-307100	7
Fagron	Cloridrato de clortetraciclina	14J08-B07-307742	4
Fagron	Cloridrato de clortetraciclina	1604015-01	2
Fagron	Cloridrato de clortetraciclina	16b10-b09	1
Fagron	Cloridrato de clortetraciclina	16B10-B09	7
Fagron	Cloridrato de clortetraciclina	16B10-B09-318088	5
Fagron	Cloridrato de clortetraciclina	16B10-B09-320304	6
Fagron	Cloridrato de clortetraciclina	16B10-B09-322715	5
Fagron	Cloridrato de clortetraciclina	16B10-B09-322716	2
Fagron	Cloridrato de clortetraciclina	16B10-B09-326865	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de clortetraciclina	16B10-B09-329778	2
Fagron	Cloridrato de clortetraciclina	16B10-B09-331443	1
Fagron	Cloridrato de clortetraciclina	16b10-b09-336332	1
Fagron	Cloridrato de clortetraciclina	16B10-B09-336332	10
Fagron	Cloridrato de clortetraciclina	16B10-B09-342410	2
Fagron	Cloridrato de clortetraciclina	16b10b09347439	1
Fagron	Cloridrato de clortetraciclina	16B10-B09-348359	1
Fagron	Cloridrato de clortetraciclina	16B10-B09-351565	4
Fagron	Cloridrato de clortetraciclina	16B10-B09-352970	6
Fagron	Cloridrato de clortetraciclina	16b10b09355611	1
Fagron	Cloridrato de clortetraciclina	1803037-01	2
Fagron	Cloridrato de clortetraciclina	1803037-03	2
Fagron	Cloridrato de clortetraciclina	1910002-01	2
Fagron	Cloridrato de clortetraciclina	191002-01	1
Fagron	Cloridrato de clortetraciclina	27121306	1
Fagron	Cloridrato de clortetraciclina	3918Q-01155	1
Fagron	Cloridrato de clortetraciclina	5014M-01155T	1
Fagron	Cloridrato de clortetraciclina	700156-B09-347439	1
Fagron	Cloridrato de clortetraciclina	FC11051038	1
Fagron	Cloridrato de clortetraciclina	FC13030134	1
Fagron	Cloridrato de clortetraciclina	FC15100204	5
Fiebig/EuRho	Cloridrato de clortetraciclina	1910002-01	1
Fiebig	Cloridrato de clortetraciclina	1412008-01	1
Fiebig	Cloridrato de clortetraciclina	1604015-01	1
Fiebig	Cloridrato de clortetraciclina	1910002-02	2
Fiebig	Cloridrato de clortetraciclina	FC15100204	1
Fragon/Sanacorp	Cloridrato de clortetraciclina	16B10-B09-352970	1
Fuijan/Noweda	Cloridrato de clortetraciclina	FC17090368	1
Fuijan/Noweda	Cloridrato de clortetraciclina	FC19040113	2
Fujan Pharmaceutic	Cloridrato de clortetraciclina	2009026-01	3
Fujang Fukang China	Cloridrato de clortetraciclina	200902601	1
Fujian Fukang Phamaceutic	Cloridrato de clortetraciclina	2205011-01	1
Fujian Fukang/Phoenix	Cloridrato de clortetraciclina	2009026-01	3
Gehe/Fagro	Cloridrato de clortetraciclina	16B10-B09-338800	1
GEHE	Cloridrato de clortetraciclina	1604015-01	1
Gehe	Cloridrato de clortetraciclina	16B10-B09	2
Gehe	Cloridrato de clortetraciclina	16B10-B09-322715	1
Gehe	Cloridrato de clortetraciclina	16B10-B09-322716	1
Gehe	Cloridrato de clortetraciclina	1910002-02	1
Gehe	Cloridrato de clortetraciclina	2205011-01	1
Geibo/Euro11.06.19	Cloridrato de clortetraciclina	1803037-01	1
Krieger	Cloridrato de clortetraciclina	12C16-No1	1
Nachprüfung 2574	Cloridrato de clortetraciclina	1108051-01	1
Nachprüfung	Cloridrato de clortetraciclina	1108051-01	1
Noweda	Cloridrato de clortetraciclina	12c16-n01	1
Noweda	Cloridrato de clortetraciclina	1412008-01	1
Noweda	Cloridrato de clortetraciclina	160401501	1
Noweda	Cloridrato de clortetraciclina	1803037	1
Noweda	Cloridrato de clortetraciclina	1803037-01	1
Noweda	Cloridrato de clortetraciclina	1910002-02	2
Noweda	Cloridrato de clortetraciclina	2205011-01	1
Noweda	Cloridrato de clortetraciclina	EurootcPharama	1
Noweda	Cloridrato de clortetraciclina	EuroOTCPharma	1
Phoenix	Cloridrato de clortetraciclina	110805102	1
Phoenix	Cloridrato de clortetraciclina	16B10-B09-322716	1
Phoenix	Cloridrato de clortetraciclina	1803037-01	1
Phoenix	Cloridrato de clortetraciclina	3407	1
Phönix/apo ident	Cloridrato de clortetraciclina	1604015-01	1
Phönix/EurHo	Cloridrato de clortetraciclina	1803037-01	1
Phönix/EurHo	Cloridrato de clortetraciclina	191000201	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix/Euro	Cloridrato de clortetraciclina	180303701	2
Phönix/EuRo	Cloridrato de clortetraciclina	1910002-02	1
Phönix	Cloridrato de clortetraciclina	1108051-02	2
Phönix	Cloridrato de clortetraciclina	1412008-01	1
phönix	Cloridrato de clortetraciclina	16B10-B09-336332	1
Phönix	Cloridrato de clortetraciclina	1803037	1
Phönix	Cloridrato de clortetraciclina	1803037-03	1
Phönix	Cloridrato de clortetraciclina	FC17090368	1
Sanacop	Cloridrato de clortetraciclina	1412008-02	1
Sanacorp	Cloridrato de clortetraciclina	1108051-01	1
Sanacorp	Cloridrato de clortetraciclina	14J08-B07	1
Sanacorp	Cloridrato de clortetraciclina	1604015-01	1
Sanacorp	Cloridrato de clortetraciclina	16B10-B09	1
Sanacorp	Cloridrato de clortetraciclina	180303701	1
Sanacorp	Cloridrato de clortetraciclina	FC15100204	1

- 235 394 spectra from 1515 *Apo-Ident* customers from a total of 49 157 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de clortetraciclina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de clortetraciclina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	190	0	201 894
Type C	0	662	11	235 394

The substance/substance group *Cloridrato de clortetraciclina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	98.3655 % (> 97.9198 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20845	20845	0,00	57,99
21222	20845	7,52	60,42
21241	20845	10,13	57,83
21877	22541	10,13	65,59
22541	22541	0,00	61,57
24959	24959	0,00	87,65
25573	25573	0,00	76,82
26229	26229	0,00	59,21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de cocaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21140-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de cocaína; Cocaína, cloridrato; Cocaini hydrochloridum

Special notes

When selecting the *Cloridrato de cocaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de cocaína	6	4	29

Second-stage model

For differentiation of the substance/substance group *Cloridrato de cocaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de cocaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de diltiazem	65,58	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de cocaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de cocaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de cocaína	13259305	21140	40	0814J-01278
Caelo	Cloridrato de cocaína	13259305	21140SI	60	0814J-01278
Caelo	Cloridrato de cocaína	15224802	22406	60	1316Q-01278
Caelo	Cloridrato de cocaína	15224802	22406SI	60	1316Q-01278
Caelo	Cloridrato de cocaína	15224802	22411	60	1316Q-01278
Caelo	Cloridrato de cocaína	15224802	22411SI	60	1316Q-01278
Caelo	Cloridrato de cocaína	17003902	23470	40	1917S-01278
Fagron	Cloridrato de cocaína	13I17-N02	21142	40	0814I-01278
Fagron	Cloridrato de cocaína	13I17-N02	21142SI	60	0814I-01278
Fagron	Cloridrato de cocaína	16B11-B05-323386	23471	40	1917Q-1278
Th. Geyer	Cloridrato de cocaína	60145	21144	40	0814K-01278
Th. Geyer	Cloridrato de cocaína	60145	21144SI	60	0814K-01278

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 620 spectra of 12 reference samples from the substance/substance group *Cloridrato de cocaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 342 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 10 reference samples from the substance/substance group *Cloridrato de cocaína*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de cocaína	16142710	23473	40
Caelo	Cloridrato de cocaína	18266104	24648	40
Fagron	Cloridrato de cocaína	14H27-B03-304551	23472	40
Fagron	Cloridrato de cocaína	18J01-B07-353630	24649	40
Caelo	Cloridrato de cocaína	17003902	23470SI†	40
Caelo	Cloridrato de cocaína	16142710	23473SI	40
Caelo	Cloridrato de cocaína	18266104	24648SI	40
Fagron	Cloridrato de cocaína	16B11-B05-323386	23471SI†	40
Fagron	Cloridrato de cocaína	14H27-B03-304551	23472SI	40
Fagron	Cloridrato de cocaína	18J01-B07-353630	24649SI	40

- 201 684 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 43 spectra from 16 *Apo-Ident* customers from 31 batches from the substance/substance group *Cloridrato de cocaína*.

- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de cocaína	21004044019	1
Caelo	Cloridrato de cocaína	12329103	1
Caelo	Cloridrato de cocaína	13112102	1
Caelo	Cloridrato de cocaína	13259306	1
Caelo	Cloridrato de cocaína	14069209	1
Caelo	Cloridrato de cocaína	16051402	1
Caelo	Cloridrato de cocaína	17003902	2
Caelo	Cloridrato de cocaína	17003909	1
Caelo	Cloridrato de cocaína	18256109	1
Caelo	Cloridrato de cocaína	18266104	3
Caelo	Cloridrato de cocaína	18266109	1
Caelo	Cloridrato de cocaína	18J01-B07-353630	2
Caelo	Cloridrato de cocaína	19073003	1
Caelo	Cloridrato de cocaína	20003901001	1
Caelo	Cloridrato de cocaína	21004044004	1
Caesar & Loretz GmbH...	Cloridrato de cocaína	18266109	2
Caesar & Loretz GmbH...	Cloridrato de cocaína	20003901001	1
Caesar & Loretz GmbH...	Cloridrato de cocaína	182661	1
Caesar & Loretz GmbH...	Cloridrato de cocaína	18266104	1
Caesar & Loretz GmbH	Cloridrato de cocaína	182661001	1
Caesar & Loretz GmbH	Cloridrato de cocaína	21004044009	1
Fagron	Cloridrato de cocaína	12G23-N13	1
Fagron	Cloridrato de cocaína	13G03-N08	2
Fagron	Cloridrato de cocaína	14H27-B03	1
Fagron	Cloridrato de cocaína	15-00638	1
Fagron	Cloridrato de cocaína	15E12-B03	1
Fagron	Cloridrato de cocaína	16B11-B05-323385	1
Fagron	Cloridrato de cocaína	17003902	2
Fagron	Cloridrato de cocaína	17E17-B07-335110	1
Fagron	Cloridrato de cocaína	17K28-B05-343075	1
Fagron	Cloridrato de cocaína	18J01-B07-353629	1
Fagron	Cloridrato de cocaína	21K30-F04	1
Gatt-Koller	Cloridrato de cocaína	20172282	1
Macfarlan Smith/Noweda	Cloridrato de cocaína	15224802	2
Synopharm	Cloridrato de cocaína	16B11-B05	1

- 236 024 spectra from 1515 *Apo-Ident* customers from a total of 49 227 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de cocaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de cocaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	400	0	201 684
Type C	0	42	1	236 024

The substance/substance group *Cloridrato de cocaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.9007 %)	97.6744 % (> 90.6977 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21140	21140	0,00	74,04
21142	21142	0,00	76,21
21144	21144	0,00	75,92
22406	22406	0,00	72,00
22411	22411	0,00	83,59
23470	23470	0,00	74,76
23471	23471	0,00	80,59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de difenidramina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20186-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de difenidramina; Difenidramina, cloridrato; Diphenhydramini hydrochloridum

Special notes

When selecting the *Cloridrato de difenidramina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de difenidramina	7	5	65

Second-stage model

For differentiation of the substance/substance group *Cloridrato de difenidramina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de difenidramina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de doxepina	79,41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de difenidramina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de difenidramina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de difenidramina	12329816	21304	40	20121119
Caelo	Cloridrato de difenidramina	12329816	21464	60	20121119
Caelo	Cloridrato de difenidramina	16004901	23235	40	20160122
Caelo	Cloridrato de difenidramina	180082	24755	40	20180126*
Caelo	Cloridrato de difenidramina	22002760	26361	30	20220923*
Caelo	Cloridrato de difenidramina	22002760	26361SI	20	20220923*
Fagron	Cloridrato de difenidramina	16C25-B03-331026	23262	40	AR-17-FG-015432-02
Fagron	Cloridrato de difenidramina	18K28-B02-358954	24702	40	20181219
Fagron	Cloridrato de difenidramina	20G03-F08-374141	25746	50	20200928

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Cloridrato de difenidramina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Cloridrato de difenidramina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de difenidramina	15072617	23206	40
Caelo	Cloridrato de difenidramina	172276	23803	40
Caelo	Cloridrato de difenidramina	183010	24390	40
Caelo	Cloridrato de difenidramina	22003785	26717	40
Caelo	Cloridrato de difenidramina	23001022	26836	40
Caelo	Cloridrato de difenidramina	22003785	26717SI	20
Caelo	Cloridrato de difenidramina	23001022	26836SI	20

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 206 spectra from 104 *Apo-Ident* customers from 67 batches from the substance/substance group *Cloridrato de difenidramina*.

- Among them are spectra of independent samples from 65 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de difenidramina	21000109013	1
	Cloridrato de difenidramina	22002760004	2
	Cloridrato de difenidramina	22002760007	1
	Cloridrato de difenidramina	22003785002	1
Caelo	Cloridrato de difenidramina		1
Caelo	Cloridrato de difenidramina	10122030	1
Caelo	Cloridrato de difenidramina	12007702	1
Caelo	Cloridrato de difenidramina	12007713	2
Caelo	Cloridrato de difenidramina	12007715	2
Caelo	Cloridrato de difenidramina	12007716	1
Caelo	Cloridrato de difenidramina	12007721	2
Caelo	Cloridrato de difenidramina	12329805	1
Caelo	Cloridrato de difenidramina	12329815	2
Caelo	Cloridrato de difenidramina	13100462	1
Caelo	Cloridrato de difenidramina	13331810	2
Caelo	Cloridrato de difenidramina	13331813	1
Caelo	Cloridrato de difenidramina	13343104	1
Caelo	Cloridrato de difenidramina	15072602	4
Caelo	Cloridrato de difenidramina	15072603	5
Caelo	Cloridrato de difenidramina	15072608	1
Caelo	Cloridrato de difenidramina	15072609	6
Caelo	Cloridrato de difenidramina	15072614	12
Caelo	Cloridrato de difenidramina	15072617	3
Caelo	Cloridrato de difenidramina	15072630	1
Caelo	Cloridrato de difenidramina	15220402	1
Caelo	Cloridrato de difenidramina	15220403	8
Caelo	Cloridrato de difenidramina	15220404	3
Caelo	Cloridrato de difenidramina	15220405	3
Caelo	Cloridrato de difenidramina	16004905	1
Caelo	Cloridrato de difenidramina	16004908	3
Caelo	Cloridrato de difenidramina	16004910	8
Caelo	Cloridrato de difenidramina	18008201	5
Caelo	Cloridrato de difenidramina	18008202	3
Caelo	Cloridrato de difenidramina	18008205	5
Caelo	Cloridrato de difenidramina	18008208	10
Caelo	Cloridrato de difenidramina	18108407	1
Caelo	Cloridrato de difenidramina	1814A-01339	1
Caelo	Cloridrato de difenidramina	18168403	3
Caelo	Cloridrato de difenidramina	18168407	17
Caelo	Cloridrato de difenidramina	1912I-01339	1
Caelo	Cloridrato de difenidramina	2000239001	1
Caelo	Cloridrato de difenidramina	20002393001	4
Caelo	Cloridrato de difenidramina	20071502	1
Caelo	Cloridrato de difenidramina	2041403	1
Caelo	Cloridrato de difenidramina	21000108002	1
Caelo	Cloridrato de difenidramina	21000109007	2
Caelo	Cloridrato de difenidramina	21000109013	1
Caelo	Cloridrato de difenidramina	22003785002	1
Caelo	Cloridrato de difenidramina	2215I-01339	1
Caelo	Cloridrato de difenidramina	25071306	1
Caelo	Cloridrato de difenidramina	2517M-01339	1
Caelo	Cloridrato de difenidramina	2818A-01339	1
Caelo	Cloridrato de difenidramina	3071715	1
Caelo	Cloridrato de difenidramina	31031508	1
Caelo	Cloridrato de difenidramina	5121204	1
Caelo	Cloridrato de difenidramina	8072001	1
Caeolo	Cloridrato de difenidramina	18008205	1
Caesar & Loretz GmbH...	Cloridrato de difenidramina	18168407	2
Caesar & Loretz GmbH...	Cloridrato de difenidramina	18168407	1
Caesar & Loretz GmbH...	Cloridrato de difenidramina	21000108002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH…	Cloridrato de difenidramina	21000109007	2
Caesar & Loretz GmbH	Cloridrato de difenidramina	18008208	1
Caesar & Loretz GmbH	Cloridrato de difenidramina	18168407	13
Caesar & Loretz GmbH	Cloridrato de difenidramina	20002393004	1
Caesar & Loretz GmbH	Cloridrato de difenidramina	21000108003	1
Caesar & Loretz GmbH	Cloridrato de difenidramina	21000109003	1
Caesar & Loretz GmbH	Cloridrato de difenidramina	21000109007	4
Caesar & Loretz Hilden	Cloridrato de difenidramina	16004905	1
Caesar & Loretz Hilden	Cloridrato de difenidramina	18008205	1
Caesar & Loretz Hilden	Cloridrato de difenidramina	18168403	1
Caesar & Loretz Hilden	Cloridrato de difenidramina	18168407	2
Caesar & Loretz Hilden	Cloridrato de difenidramina	20002393001	2
Caesar/Noweda	Cloridrato de difenidramina	12007714	1
Fagron	Cloridrato de difenidramina	12F28-N01	1
Fagron	Cloridrato de difenidramina	12J04-N02	1
Fagron	Cloridrato de difenidramina	13A14-B40-293346	1
Fagron	Cloridrato de difenidramina	15072614	1
Fagron	Cloridrato de difenidramina	16C25-B03-331026	1
Finze	Cloridrato de difenidramina	9F05-N04	2
Gatt-Koller	Cloridrato de difenidramina	21J02410	1
Gatt-Koller	Cloridrato de difenidramina	606030315	1
Gehe	Cloridrato de difenidramina	12329815	1
Jenne	Cloridrato de difenidramina	18008208	1
L30	Cloridrato de difenidramina	18008201	1
Noweda	Cloridrato de difenidramina	12007716	1
Noweda	Cloridrato de difenidramina	15220402	1
PHOENIX 29.01.2013	Cloridrato de difenidramina	120208	1
Phönix WE: 07.01.14 …	Cloridrato de difenidramina	12329805	1
Recordati/Noweda	Cloridrato de difenidramina	17100490	1
Sanacorp	Cloridrato de difenidramina	12329805	1
Sanacorp	Cloridrato de difenidramina	15072608	1
Sanacorp	Cloridrato de difenidramina	15072617	1
Sanacorp	Cloridrato de difenidramina	16004908	1
Supriya/Noweda	Cloridrato de difenidramina	20002393004	1

- 235 861 spectra from 1515 *Apo-Ident* customers from a total of 49 192 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de difenidramina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de difenidramina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	240	0	201 844
Type C	0	193	13	235 861

The substance/substance group *Cloridrato de difenidramina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	93.6893 % (> 92.2330 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21304	23262	18,78	102,26
21464	23262	16,09	102,07
23235	23262	17,99	101,77
23262	23262	0,00	109,33
24702	23262	9,02	107,35
24755	24755	0,00	101,41
25746	23262	10,05	102,35
26361	26361	0,00	102,31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de diltiazem**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20043-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de diltiazem; Diltiazem, cloridrato; Diltiazemi hydrochloridum

Special notes

When selecting the *Cloridrato de diltiazem* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de diltiazem	6	6	642

Second-stage model

For differentiation of the substance/substance group *Cloridrato de diltiazem* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de diltiazem* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de cocaína	72,75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de diltiazem* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de diltiazem*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de diltiazem	13346914	21300	40	20131028
Caelo	Cloridrato de diltiazem	13346914	21406	60	20131028
Caelo	Cloridrato de diltiazem	13346914	21407	60	20131028
Caelo	Cloridrato de diltiazem	161908	22631	40	20160715*
Caelo	Cloridrato de diltiazem	170432	23325	40	20170331*
Fagron	Cloridrato de diltiazem	14C12-B04	21270	40	20140417
Fagron	Cloridrato de diltiazem	16G20-B03-328133	23015	40	20160829
Fagron	Cloridrato de diltiazem	16G20-B03-328133	23016	40	20160829
Fagron	Cloridrato de diltiazem	20C12-F03-371907	25365	40	20200713

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Cloridrato de diltiazem*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 562 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 300 spectra of 9 reference samples from the substance/substance group *Cloridrato de diltiazem*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de diltiazem	173370	23826	40
Caelo	Cloridrato de diltiazem	183011	24389	40
Caelo	Cloridrato de diltiazem	190841	24505	40
Caelo	Cloridrato de diltiazem	22001215	26115	40
Caelo	Cloridrato de diltiazem	23001896	26950	40
Fagron	Cloridrato de diltiazem	23H17-B02-238695	27376	40
Caelo	Cloridrato de diltiazem	22001215	26115SI	20
Caelo	Cloridrato de diltiazem	23001896	26950SI	20
Fagron	Cloridrato de diltiazem	23H17-B02-238695	27376SI	20

- 201 784 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4555 spectra from 1143 *Apo-Ident* customers from 697 batches from the substance/substance group *Cloridrato de diltiazem*.

- Among them are spectra of independent samples from 642 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de diltiazem	135968-0009	1
	Cloridrato de diltiazem	20C12-F03-371907	1
	Cloridrato de diltiazem	21D26-F02-378333	1
	Cloridrato de diltiazem	21F11-B03-218858	2
	Cloridrato de diltiazem	21F11-B03-221071	1
	Cloridrato de diltiazem	21F11-B03-223064	2
	Cloridrato de diltiazem	21F11-BB03-221071	1
	Cloridrato de diltiazem	21F11-Bo3-221072	1
	Cloridrato de diltiazem	22/13-B07-223063	2
	Cloridrato de diltiazem	22/13-B07225364	1
	Cloridrato de diltiazem	22001215002	1
	Cloridrato de diltiazem	22001215009	1
	Cloridrato de diltiazem	22001215011	1
	Cloridrato de diltiazem	22001215012	5
	Cloridrato de diltiazem	22001215018	2
	Cloridrato de diltiazem	22001215019	9
	Cloridrato de diltiazem	22001215024	9
	Cloridrato de diltiazem	22001215026	7
	Cloridrato de diltiazem	22001215028	1
	Cloridrato de diltiazem	22001215029	20
	Cloridrato de diltiazem	22001215030	25
	Cloridrato de diltiazem	2200121512	1
	Cloridrato de diltiazem	2201215029	1
	Cloridrato de diltiazem	22113-B07-223063	2
	Cloridrato de diltiazem	22113-B07-223065	1
	Cloridrato de diltiazem	22I13-B07-223063	12
	Cloridrato de diltiazem	22I13-B07-223065	1
	Cloridrato de diltiazem	22I13-B07-225364	8
	Cloridrato de diltiazem	22I13-B07-225365	1
	Cloridrato de diltiazem	22I13-B07-225366	2
	Cloridrato de diltiazem	22I13-BO7-223063	1
	Cloridrato de diltiazem	23001896002	2
	Cloridrato de diltiazem	23001896007	8
	Cloridrato de diltiazem	23001896008	3
	Cloridrato de diltiazem	23C20-B02-227683	7
	Cloridrato de diltiazem	23C20-B02-227685	1
	Cloridrato de diltiazem	23G06-B07-232368	1
	Cloridrato de diltiazem	23G06-B07-234623	2
	Cloridrato de diltiazem	23G06-B07-2347623	1
	Cloridrato de diltiazem	23G06-B08-236814	1
	Cloridrato de diltiazem	23H17-B02-238694	1
	Cloridrato de diltiazem	24000125005	1
	Cloridrato de diltiazem	24000125006	1
	Cloridrato de diltiazem	24000125007	1
	Cloridrato de diltiazem	Az-0350522	1
	Cloridrato de diltiazem	AZ-0350522	1
	Cloridrato de diltiazem	AZ-0440321	1
	Cloridrato de diltiazem	AZ-0951022	1
	Cloridrato de diltiazem	B02-2276803	4
	Cloridrato de diltiazem	B07-2230603	1
	Cloridrato de diltiazem	Dil17052023	1
11.08.14 Phoenix	Cloridrato de diltiazem	13346901	1
AEP	Cloridrato de diltiazem	22001215013	1
AHD	Cloridrato de diltiazem	14C12-B04-292757	1
AHD	Cloridrato de diltiazem	15G20-B08-314375	1
AHD	Cloridrato de diltiazem	17043210	1
AHD	Cloridrato de diltiazem	17337017	2
AHD	Cloridrato de diltiazem	18301108	3
AHD	Cloridrato de diltiazem	18A29-B01-345623	2
AHD	Cloridrato de diltiazem	20000622010	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Cloridrato de diltiazem	21000035021	1
AHD	Cloridrato de diltiazem	22001215029	1
AHD	Cloridrato de diltiazem	22001215030	1
ALH	Cloridrato de diltiazem	15414319	1
Alliance Health	Cloridrato de diltiazem	13A02-N05	1
Alliance Healthcare	Cloridrato de diltiazem	12I12-N02	1
Alliance Healthcare	Cloridrato de diltiazem	22001215007	1
Alliance	Cloridrato de diltiazem	12133008	1
Alliance	Cloridrato de diltiazem	12133009	1
Alliance	Cloridrato de diltiazem	22I13-B07-223065	1
allianz	Cloridrato de diltiazem	15230512	1
Anzag	Cloridrato de diltiazem	13346915	1
anzag	Cloridrato de diltiazem	15414319	2
Anzag	Cloridrato de diltiazem	17043203	1
apomix	Cloridrato de diltiazem	14C12-B04-292759	1
Bomastus / Alliance ...	Cloridrato de diltiazem	17043219	1
Bombastus	Cloridrato de diltiazem	16190813	1
Caelo	Cloridrato de diltiazem		4
Caelo	Cloridrato de diltiazem	10069509	1
Caelo	Cloridrato de diltiazem	1020617/16190813	1
Caelo	Cloridrato de diltiazem	10212404	1
Caelo	Cloridrato de diltiazem	10212413	1
Caelo	Cloridrato de diltiazem	1090917/17043203	1
Caelo	Cloridrato de diltiazem	1091503	1
Caelo	Cloridrato de diltiazem	11091301	1
Caelo	Cloridrato de diltiazem	11134113	1
Caelo	Cloridrato de diltiazem	11134117	4
Caelo	Cloridrato de diltiazem	11L20-N06	1
Caelo	Cloridrato de diltiazem	12/12-N02	1
Caelo	Cloridrato de diltiazem	12051802	1
Caelo	Cloridrato de diltiazem	12133006	1
Caelo	Cloridrato de diltiazem	12133008	2
Caelo	Cloridrato de diltiazem	12133009	7
Caelo	Cloridrato de diltiazem	12133010	12
Caelo	Cloridrato de diltiazem	12133011	3
Caelo	Cloridrato de diltiazem	12133014	2
Caelo	Cloridrato de diltiazem	12133022	11
Caelo	Cloridrato de diltiazem	12133023	1
Caelo	Cloridrato de diltiazem	12133028	4
Caelo	Cloridrato de diltiazem	12133029	4
Caelo	Cloridrato de diltiazem	12176801	1
Caelo	Cloridrato de diltiazem	12176804	1
Caelo	Cloridrato de diltiazem	12177101	13
Caelo	Cloridrato de diltiazem	1250417	1
Caelo	Cloridrato de diltiazem	13031501	1
Caelo	Cloridrato de diltiazem	13102004	1
Caelo	Cloridrato de diltiazem	1319604	1
Caelo	Cloridrato de diltiazem	13196103	2
Caelo	Cloridrato de diltiazem	13196104	7
Caelo	Cloridrato de diltiazem	13196105	17
Caelo	Cloridrato de diltiazem	13196107	3
Caelo	Cloridrato de diltiazem	1334609	1
Caelo	Cloridrato de diltiazem	13346901	8
Caelo	Cloridrato de diltiazem	13346902	5
Caelo	Cloridrato de diltiazem	13346903	10
Caelo	Cloridrato de diltiazem	13346904	5
Caelo	Cloridrato de diltiazem	13346905	9
Caelo	Cloridrato de diltiazem	13346908	1
Caelo	Cloridrato de diltiazem	13346914	6
Caelo	Cloridrato de diltiazem	13346915	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de diltiazem	1396103	1
Caelo	Cloridrato de diltiazem	13A02-N05	1
Caelo	Cloridrato de diltiazem	13G16-N05	1
Caelo	Cloridrato de diltiazem	13G16-No5	1
Caelo	Cloridrato de diltiazem	13J24-B04-286569	1
Caelo	Cloridrato de diltiazem	13j24-b04-286571	1
Caelo	Cloridrato de diltiazem	13J24-B04-289432	3
Caelo	Cloridrato de diltiazem	1405904	1
Caelo	Cloridrato de diltiazem	14059133	1
Caelo	Cloridrato de diltiazem	140595	1
Caelo	Cloridrato de diltiazem	14059502	1
Caelo	Cloridrato de diltiazem	14059503	3
Caelo	Cloridrato de diltiazem	14059504	3
Caelo	Cloridrato de diltiazem	14059513	18
Caelo	Cloridrato de diltiazem	14059514	16
Caelo	Cloridrato de diltiazem	140595143	1
Caelo	Cloridrato de diltiazem	14059515	3
Caelo	Cloridrato de diltiazem	14059521	2
Caelo	Cloridrato de diltiazem	14318402	4
Caelo	Cloridrato de diltiazem	14318403	4
Caelo	Cloridrato de diltiazem	14318409	14
Caelo	Cloridrato de diltiazem	14318410	3
Caelo	Cloridrato de diltiazem	14318412	18
Caelo	Cloridrato de diltiazem	14318413	3
Caelo	Cloridrato de diltiazem	14318414	3
Caelo	Cloridrato de diltiazem	14318416	2
Caelo	Cloridrato de diltiazem	1459513	1
Caelo	Cloridrato de diltiazem	14C12-B04-292757	1
Caelo	Cloridrato de diltiazem	14C12-B04-294133	1
Caelo	Cloridrato de diltiazem	14C12-B04-294135	1
Caelo	Cloridrato de diltiazem	14g22b08299781	1
Caelo	Cloridrato de diltiazem	14G22-B08-299781	1
Caelo	Cloridrato de diltiazem	15/246/DI	1
Caelo	Cloridrato de diltiazem	15212801	11
Caelo	Cloridrato de diltiazem	15212802	8
Caelo	Cloridrato de diltiazem	15212806	2
Caelo	Cloridrato de diltiazem	1521806	1
Caelo	Cloridrato de diltiazem	15230000000000000000	1
Caelo	Cloridrato de diltiazem	15230501	7
Caelo	Cloridrato de diltiazem	15230502	14
Caelo	Cloridrato de diltiazem	15230503	12
Caelo	Cloridrato de diltiazem	15230504	3
Caelo	Cloridrato de diltiazem	15230507	5
Caelo	Cloridrato de diltiazem	15230510	3
Caelo	Cloridrato de diltiazem	15230512	17
Caelo	Cloridrato de diltiazem	15230513	1
Caelo	Cloridrato de diltiazem	15230514	3
Caelo	Cloridrato de diltiazem	15230515	1
Caelo	Cloridrato de diltiazem	15230516	1
Caelo	Cloridrato de diltiazem	152341904111	1
Caelo	Cloridrato de diltiazem	154114319	1
Caelo	Cloridrato de diltiazem	15414301	21
Caelo	Cloridrato de diltiazem	15414302	15
Caelo	Cloridrato de diltiazem	15414303	1
Caelo	Cloridrato de diltiazem	15414304	1
Caelo	Cloridrato de diltiazem	15414305	4
Caelo	Cloridrato de diltiazem	15414309	2
Caelo	Cloridrato de diltiazem	15414310	1
Caelo	Cloridrato de diltiazem	15414312	1
Caelo	Cloridrato de diltiazem	15414313	16

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de diltiazem	15414318	1
Caelo	Cloridrato de diltiazem	15414319	31
Caelo	Cloridrato de diltiazem	15414320	1
Caelo	Cloridrato de diltiazem	15414321	2
Caelo	Cloridrato de diltiazem	15435807	1
Caelo	Cloridrato de diltiazem	15B12-B01-305399	1
Caelo	Cloridrato de diltiazem	15B12-B01-305400	1
Caelo	Cloridrato de diltiazem	15B12-B01-305401	1
Caelo	Cloridrato de diltiazem	15G20B-08-312065	1
Caelo	Cloridrato de diltiazem	15G20-B08-312065	2
Caelo	Cloridrato de diltiazem	15G20-B08-314375	2
Caelo	Cloridrato de diltiazem	160415D	1
Caelo	Cloridrato de diltiazem	161908	1
Caelo	Cloridrato de diltiazem	16190801	4
Caelo	Cloridrato de diltiazem	16190805	3
Caelo	Cloridrato de diltiazem	16190806	16
Caelo	Cloridrato de diltiazem	16190807	3
Caelo	Cloridrato de diltiazem	16190810	11
Caelo	Cloridrato de diltiazem	16190813	16
Caelo	Cloridrato de diltiazem	16190814	13
Caelo	Cloridrato de diltiazem	16190815	1
Caelo	Cloridrato de diltiazem	16190817	2
Caelo	Cloridrato de diltiazem	16190818	1
Caelo	Cloridrato de diltiazem	16A18-B07-31667	1
Caelo	Cloridrato de diltiazem	16A18-B07-318732	2
Caelo	Cloridrato de diltiazem	16A18-B07-318733	1
Caelo	Cloridrato de diltiazem	16A18-B07-319570	1
Caelo	Cloridrato de diltiazem	16C14_B11_322642	1
Caelo	Cloridrato de diltiazem	16C14-B11-320849	1
Caelo	Cloridrato de diltiazem	16C14-B11-322153	2
Caelo	Cloridrato de diltiazem	16G20_B03_325903	1
Caelo	Cloridrato de diltiazem	16G20-B03-325903	3
Caelo	Cloridrato de diltiazem	16G20-B03-328133	2
Caelo	Cloridrato de diltiazem	16L19-B01-330365	3
Caelo	Cloridrato de diltiazem	170043217	1
Caelo	Cloridrato de diltiazem	1704317	1
Caelo	Cloridrato de diltiazem	170432	1
Caelo	Cloridrato de diltiazem	17043202	27
Caelo	Cloridrato de diltiazem	17043203	15
Caelo	Cloridrato de diltiazem	17043204	13
Caelo	Cloridrato de diltiazem	17043205	9
Caelo	Cloridrato de diltiazem	17043207	1
Caelo	Cloridrato de diltiazem	17043208	1
Caelo	Cloridrato de diltiazem	17043210	2
Caelo	Cloridrato de diltiazem	17043212	1
Caelo	Cloridrato de diltiazem	17043213	2
Caelo	Cloridrato de diltiazem	17043215	21
Caelo	Cloridrato de diltiazem	17043216	32
Caelo	Cloridrato de diltiazem	17043217	30
Caelo	Cloridrato de diltiazem	17043218	20
Caelo	Cloridrato de diltiazem	17043219	29
Caelo	Cloridrato de diltiazem	17043223	9
Caelo	Cloridrato de diltiazem	17043224	9
Caelo	Cloridrato de diltiazem	17043227	1
Caelo	Cloridrato de diltiazem	17043228	5
Caelo	Cloridrato de diltiazem	17043230	5
Caelo	Cloridrato de diltiazem	17053181	1
Caelo	Cloridrato de diltiazem	170602DH/16190813	1
Caelo	Cloridrato de diltiazem	170729181	1
Caelo	Cloridrato de diltiazem	17331012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de diltiazem	17332021	1
Caelo	Cloridrato de diltiazem	173327027	1
Caelo	Cloridrato de diltiazem	173337018	1
Caelo	Cloridrato de diltiazem	173337026	1
Caelo	Cloridrato de diltiazem	17337004	14
Caelo	Cloridrato de diltiazem	17337005	33
Caelo	Cloridrato de diltiazem	17337007	2
Caelo	Cloridrato de diltiazem	17337009	49
Caelo	Cloridrato de diltiazem	1733701	1
Caelo	Cloridrato de diltiazem	17337010	9
Caelo	Cloridrato de diltiazem	17337011	16
Caelo	Cloridrato de diltiazem	17337012	23
Caelo	Cloridrato de diltiazem	17337014	14
Caelo	Cloridrato de diltiazem	17337016	10
Caelo	Cloridrato de diltiazem	17337017	3
Caelo	Cloridrato de diltiazem	17337018	39
Caelo	Cloridrato de diltiazem	17337025	26
Caelo	Cloridrato de diltiazem	17337026	43
Caelo	Cloridrato de diltiazem	17337027	31
Caelo	Cloridrato de diltiazem	1733712	1
Caelo	Cloridrato de diltiazem	17D11-B11-333704	1
Caelo	Cloridrato de diltiazem	17D11-B11-333705	2
Caelo	Cloridrato de diltiazem	17D11-B11-334192	3
Caelo	Cloridrato de diltiazem	17D11-B11-334837	3
Caelo	Cloridrato de diltiazem	17H25-B01-340697	2
Caelo	Cloridrato de diltiazem	17h25-b01340699	1
Caelo	Cloridrato de diltiazem	17H25-B01-343273	1
Caelo	Cloridrato de diltiazem	180320DHC/17043218	1
Caelo	Cloridrato de diltiazem	18041802	1
Caelo	Cloridrato de diltiazem	18061511	1
Caelo	Cloridrato de diltiazem	18259501	1
Caelo	Cloridrato de diltiazem	18301108	1
Caelo	Cloridrato de diltiazem	18301109	8
Caelo	Cloridrato de diltiazem	1830111	1
Caelo	Cloridrato de diltiazem	18301110	13
Caelo	Cloridrato de diltiazem	18301111	37
Caelo	Cloridrato de diltiazem	1831110	1
Caelo	Cloridrato de diltiazem	18A29_B01_345623	1
Caelo	Cloridrato de diltiazem	18A29-B01	2
Caelo	Cloridrato de diltiazem	18A29-B01-345624	1
Caelo	Cloridrato de diltiazem	18a29-b01-347886	1
Caelo	Cloridrato de diltiazem	18A29-B01-348861	4
Caelo	Cloridrato de diltiazem	18A29-B01-352907	1
Caelo	Cloridrato de diltiazem	18A29-B01-352909	1
Caelo	Cloridrato de diltiazem	18A29-B01-348861	1
Caelo	Cloridrato de diltiazem	18H09-B03	2
Caelo	Cloridrato de diltiazem	18H09-B03-352908	1
Caelo	Cloridrato de diltiazem	18H09-B03-358917	4
Caelo	Cloridrato de diltiazem	18H09-B03-358918	1
Caelo	Cloridrato de diltiazem	18H09-B03-362596	2
Caelo	Cloridrato de diltiazem	18H09-B03-366217	1
Caelo	Cloridrato de diltiazem	18H09-B03-366218	1
Caelo	Cloridrato de diltiazem	18h09-b03-366219	1
Caelo	Cloridrato de diltiazem	1904108	1
Caelo	Cloridrato de diltiazem	190840108	1
Caelo	Cloridrato de diltiazem	190841002	9
Caelo	Cloridrato de diltiazem	190841004	3
Caelo	Cloridrato de diltiazem	190841005	25
Caelo	Cloridrato de diltiazem	190841006	33
Caelo	Cloridrato de diltiazem	190841007	30

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de diltiazem	19084103	7
Caelo	Cloridrato de diltiazem	19084104	17
Caelo	Cloridrato de diltiazem	19084105	32
Caelo	Cloridrato de diltiazem	19084106	39
Caelo	Cloridrato de diltiazem	19084107	29
Caelo	Cloridrato de diltiazem	19084108	40
Caelo	Cloridrato de diltiazem	19084110	21
Caelo	Cloridrato de diltiazem	19084110P-191028-1	1
Caelo	Cloridrato de diltiazem	19084110P-200217-2	1
Caelo	Cloridrato de diltiazem	19084111	13
Caelo	Cloridrato de diltiazem	19084115	22
Caelo	Cloridrato de diltiazem	190941007/3720	1
Caelo	Cloridrato de diltiazem	19841006	1
Caelo	Cloridrato de diltiazem	19H09-B03-366217	1
Caelo	Cloridrato de diltiazem	20000622003	16
Caelo	Cloridrato de diltiazem	20000622007	2
Caelo	Cloridrato de diltiazem	20000622008	8
Caelo	Cloridrato de diltiazem	20000622009	16
Caelo	Cloridrato de diltiazem	20000622010	37
Caelo	Cloridrato de diltiazem	20000622011	21
Caelo	Cloridrato de diltiazem	20000622014	2
Caelo	Cloridrato de diltiazem	20000622015	14
Caelo	Cloridrato de diltiazem	2000622011	1
Caelo	Cloridrato de diltiazem	2000622015	1
Caelo	Cloridrato de diltiazem	20C12-F03-371907	1
Caelo	Cloridrato de diltiazem	20C-12-F03-371907	1
Caelo	Cloridrato de diltiazem	20J01F11374760	1
Caelo	Cloridrato de diltiazem	20J01-F11-374763	1
Caelo	Cloridrato de diltiazem	210000035001	1
Caelo	Cloridrato de diltiazem	210000035012	1
Caelo	Cloridrato de diltiazem	21000035001	21
Caelo	Cloridrato de diltiazem	21000035002	30
Caelo	Cloridrato de diltiazem	21000035003	30
Caelo	Cloridrato de diltiazem	21000035004	3
Caelo	Cloridrato de diltiazem	210000350069	1
Caelo	Cloridrato de diltiazem	21000035008	8
Caelo	Cloridrato de diltiazem	21000035009	29
Caelo	Cloridrato de diltiazem	21000035010	29
Caelo	Cloridrato de diltiazem	21000035011	16
Caelo	Cloridrato de diltiazem	21000035012	18
Caelo	Cloridrato de diltiazem	21000035013	3
Caelo	Cloridrato de diltiazem	21000035016	10
Caelo	Cloridrato de diltiazem	21000035017	25
Caelo	Cloridrato de diltiazem	21000035021	9
Caelo	Cloridrato de diltiazem	21000035023	2
Caelo	Cloridrato de diltiazem	2100003509	1
Caelo	Cloridrato de diltiazem	2100003510	1
Caelo	Cloridrato de diltiazem	21000035100	1
Caelo	Cloridrato de diltiazem	21000035101	1
Caelo	Cloridrato de diltiazem	2100003517	1
Caelo	Cloridrato de diltiazem	2100003521	1
Caelo	Cloridrato de diltiazem	2100035003	2
Caelo	Cloridrato de diltiazem	2100035010	1
Caelo	Cloridrato de diltiazem	2100035017	1
Caelo	Cloridrato de diltiazem	2100035021	2
Caelo	Cloridrato de diltiazem	21D26-F02-378333	3
Caelo	Cloridrato de diltiazem	21F11-B03-221071	1
Caelo	Cloridrato de diltiazem	22000062009	1
Caelo	Cloridrato de diltiazem	22001215001	1
Caelo	Cloridrato de diltiazem	22001215003	24

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de diltiazem	22001215007	11
Caelo	Cloridrato de diltiazem	22001215008	19
Caelo	Cloridrato de diltiazem	22001215009	13
Caelo	Cloridrato de diltiazem	22001215011	5
Caelo	Cloridrato de diltiazem	22001215012	7
Caelo	Cloridrato de diltiazem	22001215013	5
Caelo	Cloridrato de diltiazem	22001215015	9
Caelo	Cloridrato de diltiazem	22001215019	5
Caelo	Cloridrato de diltiazem	22001215026	1
Caelo	Cloridrato de diltiazem	22001215029	1
Caelo	Cloridrato de diltiazem	22001215030	1
Caelo	Cloridrato de diltiazem	2200125007	1
Caelo	Cloridrato de diltiazem	2200125015	1
Caelo	Cloridrato de diltiazem	2201215008	1
Caelo	Cloridrato de diltiazem	221001215008	1
Caelo	Cloridrato de diltiazem	22L13-B07-223063	1
Caelo	Cloridrato de diltiazem	23051818	1
Caelo	Cloridrato de diltiazem	2310213562	1
Caelo	Cloridrato de diltiazem	23121402	1
Caelo	Cloridrato de diltiazem	24061706	1
Caelo	Cloridrato de diltiazem	2504140I	1
Caelo	Cloridrato de diltiazem	251422/1	1
Caelo	Cloridrato de diltiazem	261115DHC	1
Caelo	Cloridrato de diltiazem	27101706	1
Caelo	Cloridrato de diltiazem	27101803	1
Caelo	Cloridrato de diltiazem	2760181	1
Caelo	Cloridrato de diltiazem	2818A-03562	1
Caelo	Cloridrato de diltiazem	3313U-03562	1
Caelo	Cloridrato de diltiazem	3442	1
Caelo	Cloridrato de diltiazem	514I-03562	1
Caelo	Cloridrato de diltiazem	6031302	1
Caelo	Cloridrato de diltiazem	7082005	1
Caelo	Cloridrato de diltiazem	8726	1
Caelo	Cloridrato de diltiazem	DIL/M-04511	1
Caelo	Cloridrato de diltiazem	DIL/M-19911	1
Caelo	Cloridrato de diltiazem	RT297	1
Caeol/Noweda	Cloridrato de diltiazem	17337018	1
Caeolo	Cloridrato de diltiazem	17337005	2
Caesar & Lorenz GmbH	Cloridrato de diltiazem	17043218	1
Caesar & Lorenz GmbH	Cloridrato de diltiazem	190841007	1
Caesar & Loretz / AHD	Cloridrato de diltiazem	19084107	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035018	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841007	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084107	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035002	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035014	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622014	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035004	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622007	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084106	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084105	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035010	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841007	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	1908410	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841007	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035002	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841004	5
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841005	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084110	1
Caesar & Loretz GmbH/AEP	Cloridrato de diltiazem	19084107	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/AHD	Cloridrato de diltiazem	21000035010	1
Caesar & Loretz GmbH/AHD	Cloridrato de diltiazem	21000035023	1
Caesar & Loretz GmbH/AHD	Cloridrato de diltiazem	22001215026	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	22001215008	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	22001215015	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841006	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035002	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035010	1
Caesar & Loretz GmbH/E	Cloridrato de diltiazem	20000622010	1
Caesar & Loretz GmbH/E	Cloridrato de diltiazem	21000035011	1
Caesar & Loretz GmbH/E	Cloridrato de diltiazem	22001215003	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	17337027	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035017	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035021	1
Caesar & Loretz GmbH/G	Cloridrato de diltiazem	21000035003	1
Caesar & Loretz GmbH/G	Cloridrato de diltiazem	21000035017	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	190841007	2
Caesar & Loretz GmbH/GEHE	Cloridrato de diltiazem	19084105	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	19084106	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	19084107	1
Caesar & Loretz GmbH/gehe	Cloridrato de diltiazem	19084108	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	20000622010	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	20000622014	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	21000035010	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	21000035011	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	21000035017	3
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	21000035021	1
Caesar & Loretz GmbH/gehe	Cloridrato de diltiazem	22001215008	1
Caesar & Loretz GmbH/Gehe	Cloridrato de diltiazem	22001215019	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622008	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622015	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035011	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084104	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084106	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035009	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035011	1
Caesar & Loretz GmbH/K	Cloridrato de diltiazem	21000035009	1
Caesar & Loretz GmbH/Kehr	Cloridrato de diltiazem	21000035023	1
Caesar & Loretz GmbH/Kehr	Cloridrato de diltiazem	22001215011	3
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841007	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084103	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084105	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084115	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035012	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	22001215007	7
Caesar & Loretz GmbH/Ph	Cloridrato de diltiazem	19084108	1
Caesar & Loretz GmbH/Ph	Cloridrato de diltiazem	20000622009	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084108	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19268401	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622003	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622008	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622015	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035003	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035004	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035008	6
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035017	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	190841007	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084103	6
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084105	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084106	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084111	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	19084115	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622009	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	20000622010	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035003	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035009	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035011	3
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035017	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	AP220802-01	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	17337027	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	12133010	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	17043218	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	17043219	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	17337009	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	17337014	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	17337018	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	17337025	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	17337026	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	17337027	4
Caesar & Loretz GmbH	Cloridrato de diltiazem	18301109	3
Caesar & Loretz GmbH	Cloridrato de diltiazem	18301110	3
Caesar & Loretz GmbH	Cloridrato de diltiazem	18301111	8
Caesar & Loretz GmbH	Cloridrato de diltiazem	190841002	3
Caesar & Loretz GmbH	Cloridrato de diltiazem	190841005	5
Caesar & Loretz GmbH	Cloridrato de diltiazem	190841006	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	190841007	9
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084103	3
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084104	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084105	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084106	9
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084107	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084108	10
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084110	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084111	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	19084115	6
Caesar & Loretz GmbH	Cloridrato de diltiazem	19135410	4
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622003	4
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622007	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622008	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622009	8
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622010	10
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622011	10
Caesar & Loretz GmbH	Cloridrato de diltiazem	20000622015	5
Caesar & Loretz GmbH	Cloridrato de diltiazem	2000622003	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	20C12-F03	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035001	9
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035002	9
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035003	12
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035004	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035008	6
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035009	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035010	9
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035011	8
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035012	5
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035013	4
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035016	5
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035017	10
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035021	6
Caesar & Loretz GmbH	Cloridrato de diltiazem	21000035023	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de diltiazem	220001215007	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215002	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215003	8
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215007	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215008	5
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215009	8
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215011	3
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215012	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215013	4
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215015	7
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215019	4
Caesar & Loretz GmbH	Cloridrato de diltiazem	22001215030	2
Caesar & Loretz GmbH	Cloridrato de diltiazem	B03-3662107	1
Caesar & Loretz GmbH	Cloridrato de diltiazem	F03-3719008	2
Caesar & Loretz GmbH...	Cloridrato de diltiazem	21000035021	1
Caesar & Loretz GmbH...	Cloridrato de diltiazem	22001215015	1
Caesar & Loretz/Geil...	Cloridrato de diltiazem	190841006	1
Caesar & Loretz/Geil...	Cloridrato de diltiazem	20000622011	1
Caesar & Loretz/Geil...	Cloridrato de diltiazem	21000035010	1
Caesar & Loretz/Noweda	Cloridrato de diltiazem	19084108	1
Caesar & Loretz/Noweda	Cloridrato de diltiazem	21000035003	1
Caesar & Loretz	Cloridrato de diltiazem	16190806	1
Caesar & Loretz	Cloridrato de diltiazem	17043202	1
Caesar & Loretz	Cloridrato de diltiazem	17043216	1
Caesar & Loretz	Cloridrato de diltiazem	17337012	1
CAESAR & LORETZ	Cloridrato de diltiazem	19084105	1
Caesar / Gehe	Cloridrato de diltiazem	16190806	1
Caesar&Loretz GmbH /Anzag	Cloridrato de diltiazem	15414302	1
Caesar&Loretz GmbH/Anzag	Cloridrato de diltiazem	14318412	1
Caesar&Loretz GmbH	Cloridrato de diltiazem	20000622010	1
Caesar&Loretz GmbH	Cloridrato de diltiazem	20000622011	1
Caesar&Loretz GmbH	Cloridrato de diltiazem	21000035003	1
Caesar&Loretz GmbH	Cloridrato de diltiazem	21000035016	1
Caeser und Loretz GmbH	Cloridrato de diltiazem	19084108	1
Caleo/ Noweda	Cloridrato de diltiazem	17337009	2
Caleo/ Noweda	Cloridrato de diltiazem	17337027	2
Caleo/gehe	Cloridrato de diltiazem	18301111	1
Caleo	Cloridrato de diltiazem	17043202	1
Cealo/Sanacorp	Cloridrato de diltiazem	14059514	1
Cealo/Sanacorp	Cloridrato de diltiazem	190841006	1
Cealo	Cloridrato de diltiazem	22001215008	1
Chiesi/Phoenix	Cloridrato de diltiazem	15230502	1
Divis Laboratories ...	Cloridrato de diltiazem	20J01-F11_374760	1
Divis's Laboratoris ...	Cloridrato de diltiazem	AZ-0560718	2
EuRho/Phönix	Cloridrato de diltiazem	14059514	1
Euro OTC	Cloridrato de diltiazem	16A18B07	1
Euro OTC	Cloridrato de diltiazem	17043216	1
Euro OTC	Cloridrato de diltiazem	17043228	1
Euro OTC	Cloridrato de diltiazem	17337005	1
Euro OTC	Cloridrato de diltiazem	17337027	1
Europharm / Gehe	Cloridrato de diltiazem	17H25-B01-343273	1
Fagon/Noweda	Cloridrato de diltiazem	18H09-B03-354798	1
Fagron	Cloridrato de diltiazem		2
Fagron	Cloridrato de diltiazem	10808-N01	1
Fagron	Cloridrato de diltiazem	10D28-N23	1
Fagron	Cloridrato de diltiazem	11-01-N08	1
Fagron	Cloridrato de diltiazem	11C14-N18	1
Fagron	Cloridrato de diltiazem	11E18-N04	3
Fagron	Cloridrato de diltiazem	11I01-N08	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de diltiazem	11J28-N05	1
Fagron	Cloridrato de diltiazem	12/12-N02	4
Fagron	Cloridrato de diltiazem	12/12-NO2	1
Fagron	Cloridrato de diltiazem	12d05-n07	1
Fagron	Cloridrato de diltiazem	12D05-N07	14
Fagron	Cloridrato de diltiazem	12D05-N070	1
Fagron	Cloridrato de diltiazem	12F19-N10	3
Fagron	Cloridrato de diltiazem	12F19-N100102/574	1
Fagron	Cloridrato de diltiazem	12I12-N02	2
Fagron	Cloridrato de diltiazem	12K07-N02	2
Fagron	Cloridrato de diltiazem	12l12-N02	1
Fagron	Cloridrato de diltiazem	13346902	1
Fagron	Cloridrato de diltiazem	13346915	1
Fagron	Cloridrato de diltiazem	135968-0009	2
Fagron	Cloridrato de diltiazem	13a02-n05	1
Fagron	Cloridrato de diltiazem	13A02N05	3
Fagron	Cloridrato de diltiazem	13A02-N05	9
Fagron	Cloridrato de diltiazem	13C14-B11-322642	1
Fagron	Cloridrato de diltiazem	13F13-N05	10
Fagron	Cloridrato de diltiazem	13G16_N05	1
Fagron	Cloridrato de diltiazem	13G16-N05	23
Fagron	Cloridrato de diltiazem	13J24-B04	3
Fagron	Cloridrato de diltiazem	13j24-b04-286569	1
Fagron	Cloridrato de diltiazem	13J24B04286569	3
Fagron	Cloridrato de diltiazem	13J24-B04-286569	11
Fagron	Cloridrato de diltiazem	13J24-B04-286570	1
Fagron	Cloridrato de diltiazem	13J24-B04-286571	2
Fagron	Cloridrato de diltiazem	14C12_B04_292757	1
Fagron	Cloridrato de diltiazem	14C12_B04-294133	1
Fagron	Cloridrato de diltiazem	14C12B04	1
Fagron	Cloridrato de diltiazem	14C12-B04	7
Fagron	Cloridrato de diltiazem	14C12-B04_294133	1
Fagron	Cloridrato de diltiazem	14C12-B04-292757	23
Fagron	Cloridrato de diltiazem	14c12-b04-292759	1
Fagron	Cloridrato de diltiazem	14C12-B04-292759	4
Fagron	Cloridrato de diltiazem	14C12-B04294133	1
Fagron	Cloridrato de diltiazem	14C12-B04-294133	6
Fagron	Cloridrato de diltiazem	14c12-b04-294134	1
Fagron	Cloridrato de diltiazem	14C12-B04-294134	1
Fagron	Cloridrato de diltiazem	14C12-B04-294135	2
Fagron	Cloridrato de diltiazem	14G22B08	1
Fagron	Cloridrato de diltiazem	14G22-B08	3
Fagron	Cloridrato de diltiazem	14g22-b08-299781	1
Fagron	Cloridrato de diltiazem	14G22-B08299781	2
Fagron	Cloridrato de diltiazem	14G22-B08-299781	13
Fagron	Cloridrato de diltiazem	14G22-B08-299782	6
Fagron	Cloridrato de diltiazem	14G22-B08-299783	1
Fagron	Cloridrato de diltiazem	15414313	1
Fagron	Cloridrato de diltiazem	15B12/B01305399	1
Fagron	Cloridrato de diltiazem	15B12-b01	1
Fagron	Cloridrato de diltiazem	15B12-B01	8
Fagron	Cloridrato de diltiazem	15B12-B01_305399	1
Fagron	Cloridrato de diltiazem	15B12-B01-305299	1
Fagron	Cloridrato de diltiazem	15b12-b01-305399	2
Fagron	Cloridrato de diltiazem	15B12B01305399	2
Fagron	Cloridrato de diltiazem	15B12-B01-305399	26
Fagron	Cloridrato de diltiazem	15b12-b01-305400	2
Fagron	Cloridrato de diltiazem	15B12B01305400	1
Fagron	Cloridrato de diltiazem	15B12-B01-305400	8
Fagron	Cloridrato de diltiazem	15B12-B01-305401	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de diltiazem	15G20-B02-310792	1
Fagron	Cloridrato de diltiazem	15G20-B08	3
Fagron	Cloridrato de diltiazem	15G20-B08-310792	1
Fagron	Cloridrato de diltiazem	15G20-B08-312065	13
Fagron	Cloridrato de diltiazem	15g20-b08-314375	1
Fagron	Cloridrato de diltiazem	15G20-B08-314375	7
Fagron	Cloridrato de diltiazem	16A14-B11-322153	1
Fagron	Cloridrato de diltiazem	16A18-B07	5
Fagron	Cloridrato de diltiazem	16A18B07316667	1
Fagron	Cloridrato de diltiazem	16A18-B07-316667	13
Fagron	Cloridrato de diltiazem	16A18B07316668	1
Fagron	Cloridrato de diltiazem	16a18-b07-318732	2
Fagron	Cloridrato de diltiazem	16A18-B07318732	1
Fagron	Cloridrato de diltiazem	16A18-B07-318732	16
Fagron	Cloridrato de diltiazem	16A18-B07-318733	3
Fagron	Cloridrato de diltiazem	16A18-B07-319570	3
Fagron	Cloridrato de diltiazem	16C14-B11	4
Fagron	Cloridrato de diltiazem	16c14-b11-211642	1
Fagron	Cloridrato de diltiazem	16C14B11320568	2
Fagron	Cloridrato de diltiazem	16C14-B11-320568	5
Fagron	Cloridrato de diltiazem	16c14-b11-320849	1
Fagron	Cloridrato de diltiazem	16C14B11320849	1
Fagron	Cloridrato de diltiazem	16C14-B11-320849	16
Fagron	Cloridrato de diltiazem	16c14-b11-322152	1
Fagron	Cloridrato de diltiazem	16C14B11322152	1
Fagron	Cloridrato de diltiazem	16C14-B11-322152	7
Fagron	Cloridrato de diltiazem	16C14-B11-322153	6
Fagron	Cloridrato de diltiazem	16C14-B11-322642	16
Fagron	Cloridrato de diltiazem	16G20-B03	4
Fagron	Cloridrato de diltiazem	16g20-b03-325903	1
Fagron	Cloridrato de diltiazem	16G20B03325903	1
Fagron	Cloridrato de diltiazem	16G20B03-325903	1
Fagron	Cloridrato de diltiazem	16G20-B03-325903	21
Fagron	Cloridrato de diltiazem	16G20-B03-328133	11
Fagron	Cloridrato de diltiazem	16G20-B03-328253	4
Fagron	Cloridrato de diltiazem	16GH20-B03-325903	1
Fagron	Cloridrato de diltiazem	16L19-B01	1
Fagron	Cloridrato de diltiazem	16L19-B01_330396	1
Fagron	Cloridrato de diltiazem	16l19-b01-330365	1
Fagron	Cloridrato de diltiazem	16L19-B01-330365	9
Fagron	Cloridrato de diltiazem	16L19-B01-330395	2
Fagron	Cloridrato de diltiazem	16L19B01330396	1
Fagron	Cloridrato de diltiazem	16L19-B01-330396	8
Fagron	Cloridrato de diltiazem	17043203	1
Fagron	Cloridrato de diltiazem	17043215	1
Fagron	Cloridrato de diltiazem	17337026	1
Fagron	Cloridrato de diltiazem	17D11-B11	6
Fagron	Cloridrato de diltiazem	17D11-B11-333704	16
Fagron	Cloridrato de diltiazem	17D-11-B11-333704	1
Fagron	Cloridrato de diltiazem	17D11-B11-333705	3
Fagron	Cloridrato de diltiazem	17D11-B11-334192	4
Fagron	Cloridrato de diltiazem	17d11b11334837	1
Fagron	Cloridrato de diltiazem	17D11-B11-334837	19
Fagron	Cloridrato de diltiazem	17d11-b11-336727	1
Fagron	Cloridrato de diltiazem	17D11B11336727	1
Fagron	Cloridrato de diltiazem	17D11-B11-336727	7
Fagron	Cloridrato de diltiazem	17H25-B01	5
Fagron	Cloridrato de diltiazem	17H25-B01-340697	18
Fagron	Cloridrato de diltiazem	17H25-B01-340698	5
Fagron	Cloridrato de diltiazem	17H25-B01-340699	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de diltiazem	17h25-b01-341596	1
Fagron	Cloridrato de diltiazem	17H25-B01341596	1
Fagron	Cloridrato de diltiazem	17H25-B01-341596	16
Fagron	Cloridrato de diltiazem	17H25-B01-341597	3
Fagron	Cloridrato de diltiazem	17H25B01-341598	1
Fagron	Cloridrato de diltiazem	17H25-B01-341598	2
Fagron	Cloridrato de diltiazem	17H25-B01-343272	1
Fagron	Cloridrato de diltiazem	17H25-B01-343273	11
Fagron	Cloridrato de diltiazem	17H25-Bo1-340697	1
Fagron	Cloridrato de diltiazem	18301110	2
Fagron	Cloridrato de diltiazem	18A29_B01_348861	1
Fagron	Cloridrato de diltiazem	18A29-01-347886	1
Fagron	Cloridrato de diltiazem	18A29-B01	16
Fagron	Cloridrato de diltiazem	18A-29-B01	1
Fagron	Cloridrato de diltiazem	18A29-B01-32907	1
Fagron	Cloridrato de diltiazem	18a29b01345623	1
Fagron	Cloridrato de diltiazem	18A29-B01-345623	17
Fagron	Cloridrato de diltiazem	18a29-b01-345624	1
Fagron	Cloridrato de diltiazem	18A29-B01-345624	1
Fagron	Cloridrato de diltiazem	18A29-B01-345625	2
Fagron	Cloridrato de diltiazem	18A29-B01-346694	12
Fagron	Cloridrato de diltiazem	18A29-B01-346695	4
Fagron	Cloridrato de diltiazem	18A29B01347886	2
Fagron	Cloridrato de diltiazem	18A29-B01-347886	22
Fagron	Cloridrato de diltiazem	18A29-B01-347887	5
Fagron	Cloridrato de diltiazem	18a29-b01-348861	1
Fagron	Cloridrato de diltiazem	18A29B01348861	2
Fagron	Cloridrato de diltiazem	18A29-B01-348861	29
Fagron	Cloridrato de diltiazem	18A29B01350964	1
Fagron	Cloridrato de diltiazem	18A29-B01-350964	5
Fagron	Cloridrato de diltiazem	18A29B01-352722	1
Fagron	Cloridrato de diltiazem	18A29-B01-352722	3
Fagron	Cloridrato de diltiazem	18A-29-B01-352722	1
Fagron	Cloridrato de diltiazem	18A29-B01-352723	6
Fagron	Cloridrato de diltiazem	18A29-B01-352907	18
Fagron	Cloridrato de diltiazem	18A29-B01-352909	4
Fagron	Cloridrato de diltiazem	18A29-B01-358861	1
Fagron	Cloridrato de diltiazem	18A29-Bo1-345623	1
Fagron	Cloridrato de diltiazem	18A-B01	1
Fagron	Cloridrato de diltiazem	18A-B01-352907	1
Fagron	Cloridrato de diltiazem	18H03-B03-358920	1
Fagron	Cloridrato de diltiazem	18H09_B03_354798	1
Fagron	Cloridrato de diltiazem	18H09_B03_358918	1
Fagron	Cloridrato de diltiazem	18H09_B03_362595	1
Fagron	Cloridrato de diltiazem	18H09-B03	32
Fagron	Cloridrato de diltiazem	18H09-B03_354798	1
Fagron	Cloridrato de diltiazem	18H09-B03_366219	1
Fagron	Cloridrato de diltiazem	18H09-B03-0008	1
Fagron	Cloridrato de diltiazem	18H09-B03-326596	1
Fagron	Cloridrato de diltiazem	18H09-B03-352908	2
Fagron	Cloridrato de diltiazem	18H09-B03-354798	20
Fagron	Cloridrato de diltiazem	18H09-B03-357183	8
Fagron	Cloridrato de diltiazem	18H09B03357184	2
Fagron	Cloridrato de diltiazem	18H09-B03-357184	5
Fagron	Cloridrato de diltiazem	18h09-b03-358917	1
Fagron	Cloridrato de diltiazem	18H09-b03-358917	1
Fagron	Cloridrato de diltiazem	18H09B03358917	1
Fagron	Cloridrato de diltiazem	18H09-B03-358917	33
Fagron	Cloridrato de diltiazem	18H-09-B03-358917	2
Fagron	Cloridrato de diltiazem	18h09b03358918	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de diltiazem	18H09B03358918	1
Fagron	Cloridrato de diltiazem	18H09-B03-358918	20
Fagron	Cloridrato de diltiazem	18H09B03358919	1
Fagron	Cloridrato de diltiazem	18H09B03-358919	1
Fagron	Cloridrato de diltiazem	18H09-B03-358919	9
Fagron	Cloridrato de diltiazem	18H09B03358920	2
Fagron	Cloridrato de diltiazem	18H09-B03-358920	5
Fagron	Cloridrato de diltiazem	18H09-B03-3589818	1
Fagron	Cloridrato de diltiazem	18H09-B03-3625905	1
Fagron	Cloridrato de diltiazem	18H09-B03-3625909	1
Fagron	Cloridrato de diltiazem	18h09-b03-362595	1
Fagron	Cloridrato de diltiazem	18H09-B03-362595	29
Fagron	Cloridrato de diltiazem	18H09B03-362596	1
Fagron	Cloridrato de diltiazem	18H09-B03-362596	22
Fagron	Cloridrato de diltiazem	18H09-B03-362596/AZ-0560718	1
Fagron	Cloridrato de diltiazem	18h09-b03-362599	2
Fagron	Cloridrato de diltiazem	18H09-B03362599	1
Fagron	Cloridrato de diltiazem	18H09-B03-362599	14
Fagron	Cloridrato de diltiazem	18H09-B03-362600	3
Fagron	Cloridrato de diltiazem	18H09B03366217	2
Fagron	Cloridrato de diltiazem	18H09-B03-366217	47
Fagron	Cloridrato de diltiazem	18-H09-B03-366217	1
Fagron	Cloridrato de diltiazem	18H09-B03366218	1
Fagron	Cloridrato de diltiazem	18H09-B03-366218	12
Fagron	Cloridrato de diltiazem	18-H09B03366218	1
Fagron	Cloridrato de diltiazem	18H09-B03-366219	8
Fagron	Cloridrato de diltiazem	18H09-B03-58918	1
Fagron	Cloridrato de diltiazem	18H09-B03-654798	1
Fagron	Cloridrato de diltiazem	18H09-BO3-354798	1
Fagron	Cloridrato de diltiazem	18H09-BO3-362596	1
Fagron	Cloridrato de diltiazem	18H09-BO3-366218	1
Fagron	Cloridrato de diltiazem	18H19-B03-358918	2
Fagron	Cloridrato de diltiazem	18H-B03	1
Fagron	Cloridrato de diltiazem	18HO9-B03-366219	1
Fagron	Cloridrato de diltiazem	190312702	1
Fagron	Cloridrato de diltiazem	190841308	1
Fagron	Cloridrato de diltiazem	19H09-B03-357184	1
Fagron	Cloridrato de diltiazem	20C12F03	1
Fagron	Cloridrato de diltiazem	20C12-F03	11
Fagron	Cloridrato de diltiazem	20C12-F03_371907	1
Fagron	Cloridrato de diltiazem	20C12-F03-3719007	1
Fagron	Cloridrato de diltiazem	20c12f03371907	1
Fagron	Cloridrato de diltiazem	20c12-f03-371907	1
Fagron	Cloridrato de diltiazem	20C12F03371907	1
Fagron	Cloridrato de diltiazem	20C12-F03-371907	38
Fagron	Cloridrato de diltiazem	20C12-F03-371908	4
Fagron	Cloridrato de diltiazem	20C12-F03-3733809	1
Fagron	Cloridrato de diltiazem	20C12F03373389	1
Fagron	Cloridrato de diltiazem	20C12-F03-373389	6
Fagron	Cloridrato de diltiazem	20c12-f03-374171	2
Fagron	Cloridrato de diltiazem	20c12-F03-374171	1
Fagron	Cloridrato de diltiazem	20C12F03374171	1
Fagron	Cloridrato de diltiazem	20C12-F03-374171	14
Fagron	Cloridrato de diltiazem	20C12-FO3-371907	3
Fagron	Cloridrato de diltiazem	20J01-F11	5
Fagron	Cloridrato de diltiazem	20j01-f11-374760	3
Fagron	Cloridrato de diltiazem	20j01-F11-374760	1
Fagron	Cloridrato de diltiazem	20J01-F11-374760	29
Fagron	Cloridrato de diltiazem	20J01-F11-3747600	1
Fagron	Cloridrato de diltiazem	20J01F11374761	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de diltiazem	20J01-F11-374761	11
Fagron	Cloridrato de diltiazem	20J01-F11374763	1
Fagron	Cloridrato de diltiazem	20J01-F11-374763	7
Fagron	Cloridrato de diltiazem	20J01-F11-374764	12
Fagron	Cloridrato de diltiazem	20J01-F11-374765	1
Fagron	Cloridrato de diltiazem	212F11-803-216679	1
Fagron	Cloridrato de diltiazem	21D26-F02	3
Fagron	Cloridrato de diltiazem	21D26-F02-378333	32
Fagron	Cloridrato de diltiazem	21D26-F03-378339	3
Fagron	Cloridrato de diltiazem	21F11	1
Fagron	Cloridrato de diltiazem	21F11_b03_216679	1
Fagron	Cloridrato de diltiazem	21F11-803	1
Fagron	Cloridrato de diltiazem	21F11-803-216679	1
Fagron	Cloridrato de diltiazem	21F11-b03	1
Fagron	Cloridrato de diltiazem	21F11-B03	8
Fagron	Cloridrato de diltiazem	21F11-B03_221072	1
Fagron	Cloridrato de diltiazem	21F11-B03-213610	5
Fagron	Cloridrato de diltiazem	21F11-B03-213611	12
Fagron	Cloridrato de diltiazem	21F11-B03-216679	31
Fagron	Cloridrato de diltiazem	21F11B03216762	2
Fagron	Cloridrato de diltiazem	21F11-B03-216762	10
Fagron	Cloridrato de diltiazem	21F11-B03-218832	3
Fagron	Cloridrato de diltiazem	21F11-B03-218858	7
Fagron	Cloridrato de diltiazem	21F11-B03-218922	4
Fagron	Cloridrato de diltiazem	21F11-B03-2210071	1
Fagron	Cloridrato de diltiazem	21F11-B03-221071	22
Fagron	Cloridrato de diltiazem	21F11-B03-221072	1
Fagron	Cloridrato de diltiazem	21F11-B03-221073	1
Fagron	Cloridrato de diltiazem	21F11-B03-223064	7
Fagron	Cloridrato de diltiazem	21f11-bo3-216679	1
Fagron	Cloridrato de diltiazem	21F11-BO3-216679	1
Fagron	Cloridrato de diltiazem	21F11-BO3-216762	2
Fagron	Cloridrato de diltiazem	22/13-B07-223063	1
Fagron	Cloridrato de diltiazem	22082014A	1
Fagron	Cloridrato de diltiazem	22113-B07	1
Fagron	Cloridrato de diltiazem	22113-B07-223063	1
Fagron	Cloridrato de diltiazem	2213-B07-223063	1
Fagron	Cloridrato de diltiazem	221D-F02-378333	1
Fagron	Cloridrato de diltiazem	22I12-B07-223063	1
Fagron	Cloridrato de diltiazem	22I13-B07	1
Fagron	Cloridrato de diltiazem	22i13-B07-223063	1
Fagron	Cloridrato de diltiazem	22I13-B07-223063	13
Fagron	Cloridrato de diltiazem	22I13-B07-223065	5
Fagron	Cloridrato de diltiazem	22I13-B07-225364	1
Fagron	Cloridrato de diltiazem	22l13-B07	1
Fagron	Cloridrato de diltiazem	23C20-B02-227683	1
Fagron	Cloridrato de diltiazem	23C20-B02-228330	2
Fagron	Cloridrato de diltiazem	2798	1
Fagron	Cloridrato de diltiazem	3046333	1
Fagron	Cloridrato de diltiazem	362596	1
Fagron	Cloridrato de diltiazem	3713M-03562	1
Fagron	Cloridrato de diltiazem	371907	1
Fagron	Cloridrato de diltiazem	612213562	1
Fagron	Cloridrato de diltiazem	9J14-N17	1
Fagron	Cloridrato de diltiazem	AT-0810520	1
Fagron	Cloridrato de diltiazem	AZ-0100716	1
Fagron	Cloridrato de diltiazem	AZ-0150120	4
Fagron	Cloridrato de diltiazem	AZ-0350522	2
Fagron	Cloridrato de diltiazem	AZ-0440321	4
Fagron	Cloridrato de diltiazem	AZ-0440321/21F11-B03-221071	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de diltiazem	AZ-04600321	1
Fagron	Cloridrato de diltiazem	AZ-0460321	4
Fagron	Cloridrato de diltiazem	AZ-0470321	1
Fagron	Cloridrato de diltiazem	AZ0560718	1
Fagron	Cloridrato de diltiazem	AZ-0560718	18
Fagron	Cloridrato de diltiazem	AZ-0631216	10
Fagron	Cloridrato de diltiazem	AZ-0641216	4
Fagron	Cloridrato de diltiazem	az-0810520	1
Fagron	Cloridrato de diltiazem	AZ-0810520	9
Fagron	Cloridrato de diltiazem	AZ3500522	1
Fagron	Cloridrato de diltiazem	AZ-C150120	1
Fagron	Cloridrato de diltiazem	B03_2167602	1
Fagron	Cloridrato de diltiazem	B03-3625909	1
Fagron	Cloridrato de diltiazem	B03-3662107	4
Fagron	Cloridrato de diltiazem	B03-3662108	4
Fagron	Cloridrato de diltiazem	B07-2230603	1
Fagron	Cloridrato de diltiazem	Bo3-3626000	1
Fagron	Cloridrato de diltiazem	DIL/M-01314	1
Fagron	Cloridrato de diltiazem	DIL/M-0314	1
Fagron	Cloridrato de diltiazem	DIL/M-10515	2
Fagron	Cloridrato de diltiazem	DIL/M-13114	1
Fagron	Cloridrato de diltiazem	DIL/M-20215	1
Fagron	Cloridrato de diltiazem	DIL/M-21816	4
Fagron	Cloridrato de diltiazem	Dilt09122022	1
Fagron	Cloridrato de diltiazem	F01-3783303	1
Fagron	Cloridrato de diltiazem	F02-3783303	2
Fagron	Cloridrato de diltiazem	F03-3719007	9
Fagron	Cloridrato de diltiazem	F03-3719008	1
Fagron	Cloridrato de diltiazem	F03-3733809	1
Fagron	Cloridrato de diltiazem	F03-3741701	2
Fagron	Cloridrato de diltiazem	F03-374171	1
Fagron	Cloridrato de diltiazem	F11-3747600	5
Fagron	Cloridrato de diltiazem	F11-3747601	1
Fagron	Cloridrato de diltiazem	F11-3747603	1
Fagron	Cloridrato de diltiazem	F11-3747605	1
Fagron	Cloridrato de diltiazem	F11-374764	1
Fagron	Cloridrato de diltiazem	P-07041629/305400	1
Fagron	Cloridrato de diltiazem	P-09101821/348861	1
Fargon/AEP	Cloridrato de diltiazem	20C12-F03-371907	1
Fargon/AHD	Cloridrato de diltiazem	18A29-B01-352907	1
Fargon/Kehr	Cloridrato de diltiazem	16G20-B03-328133	1
Fargon/Krieger	Cloridrato de diltiazem	17H25-B1-340697	1
Fargon/Krieger	Cloridrato de diltiazem	18A29-B01-352907	1
Fargon/Krieger	Cloridrato de diltiazem	18H09-B03-354798	1
Fargon/Krieger	Cloridrato de diltiazem	18H09-B03-362595	1
Fargon/Noweda	Cloridrato de diltiazem	18H09-B03	1
Fargon/Phönix	Cloridrato de diltiazem	18H09-B03-358917	1
Fargon/Phönix	Cloridrato de diltiazem	20C12-F03-374171	1
Fargon/Phönix	Cloridrato de diltiazem	21F11-B03-216820	1
Fargon	Cloridrato de diltiazem	16C14-B11-320849	1
Fargon	Cloridrato de diltiazem	18A29-B01-348861	1
Fargon	Cloridrato de diltiazem	18A29-B01-352907	1
Fargon	Cloridrato de diltiazem	18H09-B03-362595	1
Fargon	Cloridrato de diltiazem	AZ-0810520	1
Fargon	Cloridrato de diltiazem	B03-3625905	1
Fargon	Cloridrato de diltiazem	F03-3719007	1
FGagron7Noweda	Cloridrato de diltiazem	B03-2136101	1
Fgron / Gehe	Cloridrato de diltiazem	17H25B01341596	1
Fiebig ek:12.27 01.08.12	Cloridrato de diltiazem	11/01-N08	1
Fiebig	Cloridrato de diltiazem	15230514	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Cloridrato de diltiazem	16G20-B03-328133	1
Fiebig	Cloridrato de diltiazem	17043227	1
Fragon/ Gehe	Cloridrato de diltiazem	18h09b03366217	1
Fragon/Alliance	Cloridrato de diltiazem	21F11-Bo3-216679	1
Fragon/Noweda	Cloridrato de diltiazem	16L19-B01-330396	1
Fragon/Sanacorp	Cloridrato de diltiazem	18H09-B03-358918	1
Gatt-Koller	Cloridrato de diltiazem	22J02643	1
Gehe amax	Cloridrato de diltiazem	18H09-B03-354798	1
Gehe amax	Cloridrato de diltiazem	18H09-B03-366218	1
Gehe amax	Cloridrato de diltiazem	190841005	2
Gehe amax	Cloridrato de diltiazem	19084106	1
Gehe	Cloridrato de diltiazem	12133009	1
Gehe	Cloridrato de diltiazem	12133022	1
Gehe	Cloridrato de diltiazem	13346915	1
Gehe	Cloridrato de diltiazem	14C12-B04-292757	1
Gehe	Cloridrato de diltiazem	14G22-B08-299781	1
Gehe	Cloridrato de diltiazem	15230503	1
Gehe	Cloridrato de diltiazem	15414319	1
Gehe	Cloridrato de diltiazem	15B12-B01-305399	2
Gehe	Cloridrato de diltiazem	16190806	1
Gehe	Cloridrato de diltiazem	16190813	1
GEHE	Cloridrato de diltiazem	16190813	1
Gehe	Cloridrato de diltiazem	16L-19-B01-330365	1
Gehe	Cloridrato de diltiazem	17043202	1
GEHE	Cloridrato de diltiazem	17043217	1
Gehe	Cloridrato de diltiazem	17043218	1
Gehe	Cloridrato de diltiazem	17043219	1
Gehe	Cloridrato de diltiazem	17337005	1
GEHE	Cloridrato de diltiazem	17337025	2
Gehe	Cloridrato de diltiazem	17337026	1
Gehe	Cloridrato de diltiazem	17337027	1
Gehe	Cloridrato de diltiazem	17D11-B11	1
Gehe	Cloridrato de diltiazem	17d11-b11-334837	1
Gehe	Cloridrato de diltiazem	18301111	1
Gehe	Cloridrato de diltiazem	18A29-B01	1
Gehe	Cloridrato de diltiazem	18A29-B01-348861	1
Gehe	Cloridrato de diltiazem	18A29-B01-352907	1
Gehe	Cloridrato de diltiazem	18H09-B03	1
Gehe	Cloridrato de diltiazem	18H09-B03-358917	1
Gehe	Cloridrato de diltiazem	18H09-B03-358918	1
Gehe	Cloridrato de diltiazem	18H09-B03-362599	1
GEHE	Cloridrato de diltiazem	19084110	1
Gehe	Cloridrato de diltiazem	20000622009	1
Gehe	Cloridrato de diltiazem	20C12-F03	1
Gehe	Cloridrato de diltiazem	20C12-F03-371907	1
Gehe	Cloridrato de diltiazem	20J01-F11-374760	1
Gehe	Cloridrato de diltiazem	21000035002	1
Gehe	Cloridrato de diltiazem	21000035016	1
Gehe	Cloridrato de diltiazem	21D26-F02-378333	1
Gehe	Cloridrato de diltiazem	21F11-B03-213610	1
Gehe	Cloridrato de diltiazem	21F11-B03-221071	2
Gehe	Cloridrato de diltiazem	22001215009	1
Gehe	Cloridrato de diltiazem	22001215012	1
GEHE	Cloridrato de diltiazem	22001215018	1
Gehe	Cloridrato de diltiazem	22001215024	1
Gehe	Cloridrato de diltiazem	22I13-B07-223063	1
GEHE	Cloridrato de diltiazem	22I13-B07-223063	1
Gehe	Cloridrato de diltiazem	23C20-B02-228330	1
Gehe	Cloridrato de diltiazem	F11-3747600	1
Geilenkirchen	Cloridrato de diltiazem	17043218	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Cloridrato de diltiazem	19084108	1
Hedinger GmbH	Cloridrato de diltiazem	16G20-B03	1
Jenne	Cloridrato de diltiazem	15414313	1
Jenne	Cloridrato de diltiazem	21000035017	1
Jenne	Cloridrato de diltiazem	22001215019	1
Jenne	Cloridrato de diltiazem	22001215030	1
Kehr	Cloridrato de diltiazem	17043228	1
Kehr	Cloridrato de diltiazem	22001215003	2
Kehr	Cloridrato de diltiazem	22001215030	2
Klenk	Cloridrato de diltiazem	18A29-B01-347886	1
Klosterring	Cloridrato de diltiazem	16190806	1
Krieger/Phönix	Cloridrato de diltiazem	AZ-0460321	1
Krieger	Cloridrato de diltiazem	22i13-B07-223063	1
Kuerzel	Cloridrato de diltiazem	13G16-N05	1
M/s.Piramal Enterpri...	Cloridrato de diltiazem	190841005	1
M/s.Piramal Enterpri...	Cloridrato de diltiazem	19084108	1
M/s/Noweda	Cloridrato de diltiazem	DIL/M-03519	4
Nachprüfung	Cloridrato de diltiazem		1
Noveda	Cloridrato de diltiazem	18A29-B01-348861	1
Noveda	Cloridrato de diltiazem	20000622011	1
Noweda 17.09.2019	Cloridrato de diltiazem	19084105	1
Noweda	Cloridrato de diltiazem	12133010	1
Noweda	Cloridrato de diltiazem	12133022	1
Noweda	Cloridrato de diltiazem	12133029	1
Noweda	Cloridrato de diltiazem	12176801	1
Noweda	Cloridrato de diltiazem	13346901	1
Noweda	Cloridrato de diltiazem	14318409	1
Noweda	Cloridrato de diltiazem	15230503	1
Noweda	Cloridrato de diltiazem	15414319	1
Noweda	Cloridrato de diltiazem	16190812	1
Noweda	Cloridrato de diltiazem	16L19-B01-330365	2
Noweda	Cloridrato de diltiazem	17334012	1
Noweda	Cloridrato de diltiazem	17337026	1
Noweda	Cloridrato de diltiazem	17D11-B11-334837	1
Noweda	Cloridrato de diltiazem	18H09B03358918	1
Noweda	Cloridrato de diltiazem	18H09-B03-362595	1
Noweda	Cloridrato de diltiazem	19084104	1
Noweda	Cloridrato de diltiazem	20000622011	1
Noweda	Cloridrato de diltiazem	20J01-F11-374760	1
Noweda	Cloridrato de diltiazem	21000035002	1
Noweda	Cloridrato de diltiazem	21000035003	1
Noweda	Cloridrato de diltiazem	21000035017	1
Noweda	Cloridrato de diltiazem	2100035010	1
Noweda	Cloridrato de diltiazem	21F11-B03	1
Noweda	Cloridrato de diltiazem	22001215007	2
Noweda	Cloridrato de diltiazem	22001215012	1
Noweda	Cloridrato de diltiazem	22001215018	1
Noweda	Cloridrato de diltiazem	22001215024	3
NOWEDA	Cloridrato de diltiazem	22001215030	1
Noweda	Cloridrato de diltiazem	2201215030	1
Noweda	Cloridrato de diltiazem	22113-B07-225364	1
Noweda	Cloridrato de diltiazem	22I13-B07-223063	1
Noweda	Cloridrato de diltiazem	22I13-B07-225364	1
Noweda	Cloridrato de diltiazem	22l13-B07-225365	1
Noweda	Cloridrato de diltiazem	24000125007	1
p&m cosmetics/gehe	Cloridrato de diltiazem	17043217	1
Phoenix 14.03.2019 15,21EUR	Cloridrato de diltiazem	18A29-B01-345623	1
phoenix	Cloridrato de diltiazem	11/01-N08	1
Phoenix	Cloridrato de diltiazem	13346902	1
Phoenix	Cloridrato de diltiazem	13346914	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
phoenix	Cloridrato de diltiazem	14318412	1
Phoenix	Cloridrato de diltiazem	15230503	1
Phoenix	Cloridrato de diltiazem	17337005	1
Phoenix	Cloridrato de diltiazem	17337018	1
Phoenix	Cloridrato de diltiazem	18h09-b03	1
Phoenix	Cloridrato de diltiazem	18H09-B03-357183	1
Phoenix	Cloridrato de diltiazem	20000622014	1
Phoenix	Cloridrato de diltiazem	200101601	1
Phoenix	Cloridrato de diltiazem	20J01-F11	1
Phoenix	Cloridrato de diltiazem	20j01-f11-374763	1
Phoenix	Cloridrato de diltiazem	21000035001	2
Phoenix	Cloridrato de diltiazem	21000035003	1
Phoenix	Cloridrato de diltiazem	21000035013	3
Phoenix	Cloridrato de diltiazem	2100035004	1
Phoenix	Cloridrato de diltiazem	22001215024	1
Phoenix	Cloridrato de diltiazem	22001215030	1
Phoenix	Cloridrato de diltiazem	22I13-B07-223063	1
Phoenix	Cloridrato de diltiazem	22l13-B07-223063	1
Phoenix	Cloridrato de diltiazem	23G06-B07-234623	1
Phoenix	Cloridrato de diltiazem	AZ-0260423	1
Phoenix	Cloridrato de diltiazem	B03-3625906	1
Phönix Gotha	Cloridrato de diltiazem	15230503	1
Phönix, Caesar&Loret…	Cloridrato de diltiazem	19084115	1
Phönix/Fagon	Cloridrato de diltiazem	16A18-B07_318732	1
Phönix/Fargon	Cloridrato de diltiazem	18H09-B03-358917	1
Phönix/Fargon	Cloridrato de diltiazem	AZ-0560718	1
Phönix/Fargon	Cloridrato de diltiazem	F03-3719007	1
Phönix	Cloridrato de diltiazem	13196106	1
Phönix	Cloridrato de diltiazem	13F13-N05	1
phönix	Cloridrato de diltiazem	14059514	1
Phönix	Cloridrato de diltiazem	15212801	1
Phönix	Cloridrato de diltiazem	15414302	1
Phönix	Cloridrato de diltiazem	15G20-B08-310792	1
phönix	Cloridrato de diltiazem	16G20-B03-328133	1
PHÖNIX	Cloridrato de diltiazem	17043215	2
Phönix	Cloridrato de diltiazem	17043219	1
PHÖNIX	Cloridrato de diltiazem	17337004	2
Phönix	Cloridrato de diltiazem	17d11-b11-334837	1
Phönix	Cloridrato de diltiazem	18A29-B01-347886	1
Phönix	Cloridrato de diltiazem	18A29-B01-348861	1
Phönix	Cloridrato de diltiazem	18h09-b03-358917	1
Phönix	Cloridrato de diltiazem	18H09-B03358917	1
Phönix	Cloridrato de diltiazem	18H09-B03-362595	1
Phönix	Cloridrato de diltiazem	18H09-B03-366217	2
Phönix	Cloridrato de diltiazem	19084106	1
Phönix	Cloridrato de diltiazem	19084108	1
PHÖNIX	Cloridrato de diltiazem	19084108	1
Phönix	Cloridrato de diltiazem	20000622015	1
Phönix	Cloridrato de diltiazem	2000622003	1
Phönix	Cloridrato de diltiazem	20C12-F03-373389	1
Phönix	Cloridrato de diltiazem	21F11B03213611	1
phönix	Cloridrato de diltiazem	21F11-B03-221071	2
Phönix	Cloridrato de diltiazem	22001215024	3
Phönix	Cloridrato de diltiazem	22001215030	2
PHönix	Cloridrato de diltiazem	22001215030	1
Phönix	Cloridrato de diltiazem	2200121530	1
Phönix	Cloridrato de diltiazem	AZ-0350522	2
Phönix	Cloridrato de diltiazem	AZ-0560718	1
Phönix	Cloridrato de diltiazem	AZ-0951022	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Cloridrato de diltiazem	b03-3625906	1
Phönix	Cloridrato de diltiazem	f11-3747600	1
Piramal Healthcare L...	Cloridrato de diltiazem	12/12-N02	1
Piramal/Noweda	Cloridrato de diltiazem	DIL/M-02820	4
Piramaral Healthcare LTD.	Cloridrato de diltiazem	12F19-N10	1
Röntgen	Cloridrato de diltiazem	18A29-B01-350964	1
Sanacop	Cloridrato de diltiazem	14059523	1
Sanacorp /Fargron	Cloridrato de diltiazem	16G20-B03-325903	1
Sanacorp WE 17.02.17...	Cloridrato de diltiazem	16190806	1
Sanacorp, 18.02.17, ...	Cloridrato de diltiazem	16190807	1
Sanacorp	Cloridrato de diltiazem	11134115	4
Sanacorp	Cloridrato de diltiazem	11134121	2
Sanacorp	Cloridrato de diltiazem	11J28-04511	1
Sanacorp	Cloridrato de diltiazem	12/12-N02	2
Sanacorp	Cloridrato de diltiazem	12133010	1
Sanacorp	Cloridrato de diltiazem	12I12-N02	1
Sanacorp	Cloridrato de diltiazem	13j24-b04-286569	1
Sanacorp	Cloridrato de diltiazem	14c12-b04-292757	1
Sanacorp	Cloridrato de diltiazem	17043217	1
Sanacorp	Cloridrato de diltiazem	17337005	1
Sanacorp	Cloridrato de diltiazem	17337009	1
Sanacorp	Cloridrato de diltiazem	17337026	2
Sanacorp	Cloridrato de diltiazem	18301111	2
Sanacorp	Cloridrato de diltiazem	18H09-B03	2
Sanacorp	Cloridrato de diltiazem	190841006	1
Sanacorp	Cloridrato de diltiazem	19084104	1
Sanacorp	Cloridrato de diltiazem	19084106	1
Sanacorp	Cloridrato de diltiazem	19084107	1
Sanacorp	Cloridrato de diltiazem	21000035003	1
Sanacorp	Cloridrato de diltiazem	21000035009	1
Sanacorp	Cloridrato de diltiazem	22001215007	2
Sanacorp	Cloridrato de diltiazem	22001215009	1
Sanacorp	Cloridrato de diltiazem	22001215012	1
Sanacorp	Cloridrato de diltiazem	22001215029	1
Sanacorp	Cloridrato de diltiazem	22I13-B07-223063	1
sanacorp	Cloridrato de diltiazem	23001896006	1
Sanacorp	Cloridrato de diltiazem	23G06-B07-234623	1
Sanacorp	Cloridrato de diltiazem	3216679	1
Sanacorp	Cloridrato de diltiazem	Fargon	1
sittig	Cloridrato de diltiazem	14G22-B08-299781	1
VDL;18.02.15;15,95EUR	Cloridrato de diltiazem	14059514	1
Wepa / Wepa	Cloridrato de diltiazem	17043218	1

- 231 512 spectra from 1515 *Apo-Ident* customers from a total of 48 565 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de diltiazem* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de diltiazem* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	300	0	201 784
Type C	0	4376	179	231 512

The substance/substance group *Cloridrato de diltiazem* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.9007 %)	96.0703 % (> 96.0044 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21270	22631	27,41	88,30
21300	22631	12,72	88,77
21406	22631	11,96	88,74
21407	22631	12,46	96,73
22631	22631	0,00	100,37
23015	23325	22,54	94,39
23016	22631	26,58	96,56
23325	23325	0,00	95,90
25365	22631	17,27	102,15

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de doxepina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005411-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de doxepina; Doxepina, cloridrato; Doxepini hydrochloridum

Special notes

When selecting the *Cloridrato de doxepina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de doxepina	5	4	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de doxepina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de doxepina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de benzidamina	81,69	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de doxepina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de doxepina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Dipharma	Cloridrato de doxepina	1909145	25812	50	20190716
Dipharma	Cloridrato de doxepina	2003479	25814	50	20200312
Dipharma	Cloridrato de doxepina	1909145	25815	50	2204026
Dipharma	Cloridrato de doxepina	2207952	26321	40	20220628
Fagron	Cloridrato de doxepina	18A30-B01-361389	25816	50	20190617
Fagron	Cloridrato de doxepina	21G23-B04-222859	26387	40	20211005

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Cloridrato de doxepina*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 682 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 13 reference samples from the substance/substance group *Cloridrato de doxepina*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Dipharma	Cloridrato de doxepina	1904946	25813	50
Dipharma	Cloridrato de doxepina	2112869	25897	50
Fagron	Cloridrato de doxepina	20C26-F01-371195	25720	40
Fagron	Cloridrato de doxepina	21G23-B05-215698	25910	40
Dipharma	Cloridrato de doxepina	1909145	25812SI†	10
Dipharma	Cloridrato de doxepina	1904946	25813SI	10
Dipharma	Cloridrato de doxepina	2003479	25814SI†	10
Dipharma	Cloridrato de doxepina	1909145	25815SI†	10
Dipharma	Cloridrato de doxepina	2112869	25897SI	10
Dipharma	Cloridrato de doxepina	2207952	26321SI†	20
Fagron	Cloridrato de doxepina	18A30-B01-361389	25816SI†	10
Fagron	Cloridrato de doxepina	21G23-B05-215698	25910SI	10
Fagron	Cloridrato de doxepina	21G23-B04-222859	26387SI†	20

- 201 794 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de doxepina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de doxepina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de doxepina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	290	0	201 794
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de doxepina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25812	25815	12,81	113,88
25814	25815	18,30	127,58
25815	25815	0,00	120,62
25816	25815	13,18	147,47
26321	25815	10,75	111,65
26387	25815	13,63	114,64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de efedrina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20993-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de efedrina; Efedrina, cloridrato; Ephedrini hydrochloridum

Special notes

When selecting the *Cloridrato de efedrina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de efedrina	6	4	67

Second-stage model

For differentiation of the substance/substance group *Cloridrato de efedrina* the following second-stage model is used:

- Submodelo 08

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de efedrina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	149,40	–
⋮	⋮	⋮
Prednisona	>50	33,07
Acetato de prednisolona	>50	51,44

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de efedrina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de efedrina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de efedrina	12017217	20993	40	1511635
Caelo	Cloridrato de efedrina	13323305	21322	40	20131113
Caelo	Cloridrato de efedrina	14378502	21803	60	20150106
Caelo	Cloridrato de efedrina	161197	22436	60	20160420*
Caelo	Cloridrato de efedrina	21000335008	25729	40	20210125
Caelo	Cloridrato de efedrina	21000335008	25729SI	40	20210125
Fagron	Cloridrato de efedrina	15H28-B02-316349	23073	40	20150924

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Cloridrato de efedrina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Cloridrato de efedrina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de efedrina	171736	23672	40
Caelo	Cloridrato de efedrina	22001784	26372	40
Caelo	Cloridrato de efedrina	23001657	26841	30
Fagron	Cloridrato de efedrina	20H07-B01-202226	25970	40
Caelo	Cloridrato de efedrina	22001784	26372SI	30
Caelo	Cloridrato de efedrina	23001657	26841SI	30
Fagron	Cloridrato de efedrina	20H07-B01-202226	25970SI	40

- 201 834 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 133 spectra from 52 *Apo-Ident* customers from 71 batches from the substance/substance group *Cloridrato de efedrina*.

- Among them are spectra of independent samples from 67 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de efedrina	22001784011	2
Anzag	Cloridrato de efedrina	18213113	1
Caelo	Cloridrato de efedrina		1
Caelo	Cloridrato de efedrina	10103425	1
Caelo	Cloridrato de efedrina	10119709	1
Caelo	Cloridrato de efedrina	11126407	1
Caelo	Cloridrato de efedrina	12017207	1
Caelo	Cloridrato de efedrina	12017209	2
Caelo	Cloridrato de efedrina	12017215	1
Caelo	Cloridrato de efedrina	12017217	1
Caelo	Cloridrato de efedrina	12017223	1
Caelo	Cloridrato de efedrina	13323302	1
Caelo	Cloridrato de efedrina	13323310	1
Caelo	Cloridrato de efedrina	13323316	1
Caelo	Cloridrato de efedrina	13323321	1
Caelo	Cloridrato de efedrina	14378502	1
Caelo	Cloridrato de efedrina	14378506	2
Caelo	Cloridrato de efedrina	14378507	1
Caelo	Cloridrato de efedrina	14378508	1
Caelo	Cloridrato de efedrina	14378510	1
Caelo	Cloridrato de efedrina	15179302	2
Caelo	Cloridrato de efedrina	151J9304	1
Caelo	Cloridrato de efedrina	16119702	3
Caelo	Cloridrato de efedrina	16119703	1
Caelo	Cloridrato de efedrina	16119704	1
Caelo	Cloridrato de efedrina	16119709	2
Caelo	Cloridrato de efedrina	16119710	1
Caelo	Cloridrato de efedrina	16119715	5
Caelo	Cloridrato de efedrina	16119715200218P301	1
Caelo	Cloridrato de efedrina	1619704	1
Caelo	Cloridrato de efedrina	1713601	1
Caelo	Cloridrato de efedrina	17173601	1
Caelo	Cloridrato de efedrina	17173604	1
Caelo	Cloridrato de efedrina	18006701	4
Caelo	Cloridrato de efedrina	18006702	1
Caelo	Cloridrato de efedrina	18006708	1
Caelo	Cloridrato de efedrina	18006709	1
Caelo	Cloridrato de efedrina	1813113	1
Caelo	Cloridrato de efedrina	1821	1
Caelo	Cloridrato de efedrina	182131002	1
Caelo	Cloridrato de efedrina	182131003	6
Caelo	Cloridrato de efedrina	18213103	6
Caelo	Cloridrato de efedrina	18213104	2
Caelo	Cloridrato de efedrina	18213105	1
Caelo	Cloridrato de efedrina	18213109	2
Caelo	Cloridrato de efedrina	18213111	1
Caelo	Cloridrato de efedrina	18213112	1
Caelo	Cloridrato de efedrina	18213113	2
Caelo	Cloridrato de efedrina	18213115	6
Caelo	Cloridrato de efedrina	192679004	2
Caelo	Cloridrato de efedrina	21000335002	1
Caelo	Cloridrato de efedrina	21000335004	3
Caelo	Cloridrato de efedrina	21000335009	1
Caelo	Cloridrato de efedrina	21000335011	1
Caelo	Cloridrato de efedrina	21000335012	2
Caelo	Cloridrato de efedrina	21000335013	1
Caelo	Cloridrato de efedrina	22001784007	1
Caesar & Loretz GmbH...	Cloridrato de efedrina	11126411	1
Caesar & Loretz GmbH	Cloridrato de efedrina	14378503	1
Caesar & Loretz GmbH	Cloridrato de efedrina	18213103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de efedrina	18213104	2
Caesar & Loretz GmbH	Cloridrato de efedrina	18213109	1
Caesar & Loretz GmbH	Cloridrato de efedrina	18213113	3
Caesar & Loretz GmbH	Cloridrato de efedrina	18213115	2
Caesar & Loretz GmbH	Cloridrato de efedrina	192679004	2
Caesar & Loretz GmbH	Cloridrato de efedrina	21000335002	1
Caesar & Loretz GmbH	Cloridrato de efedrina	21000335011	3
Caesar & Loretz GmbH	Cloridrato de efedrina	21000335012	2
Caesar & Loretz GmbH	Cloridrato de efedrina	22001784003	1
Caesar & Loretz Hilden	Cloridrato de efedrina	18213103	1
Cealo, GEHE	Cloridrato de efedrina	21000335001	1
Fagron	Cloridrato de efedrina	12017220	1
Fagron	Cloridrato de efedrina	13B19-N04	1
Fagron	Cloridrato de efedrina	13L30-B36	1
Gatt-Koller / Phoenix	Cloridrato de efedrina	18502141114	1
GATT-KOLLER/PHOENIX	Cloridrato de efedrina	915/03141314	2
Gehe am 04.03.14	Cloridrato de efedrina	13323303	1
LandSiegfried Pharma…	Cloridrato de efedrina	17242077	5
LandSiegfried Pharma…	Cloridrato de efedrina	19212002	1
Phoenix 04.03.14	Cloridrato de efedrina	1332303	1
PHOENIX 10.03.2014	Cloridrato de efedrina	13323302	1
Phönix	Cloridrato de efedrina	13323305	2
Phönix	Cloridrato de efedrina	13323315	1

- 235 934 spectra from 1515 *Apo-Ident* customers from a total of 49 188 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de efedrina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de efedrina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	210	40	201 834
Type C	0	133	0	235 934

The substance/substance group *Cloridrato de efedrina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	84.0000 % (> 82.8000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.4887 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20993	20993	0,00	214,97
21322	22436	7,50	212,83
21803	22436	4,79	213,76
22436	22436	0,00	216,41
23073	20993	5,33	214,41
25729	22436	5,88	212,80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de fenilefrina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20567-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de fenilefrina; Fenilefrina, cloridrato; Phenylephrini hydrochloridum

Special notes

When selecting the *Cloridrato de fenilefrina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de fenilefrina	8	4	87

Second-stage model

For differentiation of the substance/substance group *Cloridrato de fenilefrina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de fenilefrina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citrato de cafeína	129,54	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de fenilefrina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de fenilefrina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de fenilefrina	1704009	23394	40	20170524*
Euro OTC	Cloridrato de fenilefrina	2001012	25102	40	20200218*
Euro OTC	Cloridrato de fenilefrina	2109007	25823	50	20211006*
Euro OTC	Cloridrato de fenilefrina	2202012	26039	40	20220310*
Fagron	Cloridrato de fenilefrina	12J19-B40-288254	21051	40	20131210
Fagron	Cloridrato de fenilefrina	14H13-B02-308438	21960	60	AR-16-FG-008920-01
Fagron	Cloridrato de fenilefrina	16A20-B07-317987	22388	40	AR-16-FG-013385-01
Fagron	Cloridrato de fenilefrina	20D01-F06-370692	25366	40	20200529

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 350 spectra of 8 reference samples from the substance/substance group *Cloridrato de fenilefrina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 612 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Cloridrato de fenilefrina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de fenilefrina	2010018	25455	40
Fagron	Cloridrato de fenilefrina	17C23-B04-333878	23263	40
Fagron	Cloridrato de fenilefrina	17C23-B04-333880	23267	40
Fagron	Cloridrato de fenilefrina	22D28-B01-218602	26167	40
Euro OTC	Cloridrato de fenilefrina	2109007	25823SI†	10
Euro OTC	Cloridrato de fenilefrina	2202012	26039SI†	40
Fagron	Cloridrato de fenilefrina	22D28-B01-218602	26167SI	40

- 201 834 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 208 spectra from 38 *Apo-Ident* customers from 92 batches from the substance/substance group *Cloridrato de fenilefrina*.

- Among them are spectra of independent samples from 87 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de fenilefrina	21C04-F02-377267	1
	Cloridrato de fenilefrina	21F15-B10-216432	1
	Cloridrato de fenilefrina	23A04-B05-226165	1
ALH	Cloridrato de fenilefrina	16A20-B07-322159	1
Audor Pharma	Cloridrato de fenilefrina	APP70-16017PE	1
Audor Pharma	Cloridrato de fenilefrina	APP70-17001PE	2
Audor Pharma	Cloridrato de fenilefrina	APP70-17011PE	1
Audor Pharma	Cloridrato de fenilefrina	APP70-18008PE	1
Caelo	Cloridrato de fenilefrina	14H13-B02-308438	1
Caelo	Cloridrato de fenilefrina	17C23-B04-334819	1
Caelo	Cloridrato de fenilefrina	17H18-B02_353092	1
Caelo	Cloridrato de fenilefrina	17H18-B02-349261	2
Caelo	Cloridrato de fenilefrina	17H18-B02-353092	1
Caelo	Cloridrato de fenilefrina	18026008	1
Euro OTC	Cloridrato de fenilefrina	1704009-01	1
Euro OTC	Cloridrato de fenilefrina	2001012-01	1
Euro OTC	Cloridrato de fenilefrina	2010018-01	1
Euro OTC	Cloridrato de fenilefrina	21022182	1
Euro OTC	Cloridrato de fenilefrina	2109007-01	2
Faggron/Sanacorp	Cloridrato de fenilefrina	13K25-B02-293844	3
Fagon	Cloridrato de fenilefrina	20D01-F06-370690	1
Fagron	Cloridrato de fenilefrina	10091504	1
Fagron	Cloridrato de fenilefrina	1021402	1
Fagron	Cloridrato de fenilefrina	12031801	1
Fagron	Cloridrato de fenilefrina	12A03-N09	1
Fagron	Cloridrato de fenilefrina	12C08-N17	1
Fagron	Cloridrato de fenilefrina	12F01-N20	2
Fagron	Cloridrato de fenilefrina	12g19-n04	1
Fagron	Cloridrato de fenilefrina	12G19-N04	1
Fagron	Cloridrato de fenilefrina	12J19-B40-288253	2
Fagron	Cloridrato de fenilefrina	13A03-N09	3
Fagron	Cloridrato de fenilefrina	13B14-N03	1
Fagron	Cloridrato de fenilefrina	13G10-N04	1
Fagron	Cloridrato de fenilefrina	13K25-B02-293845	1
Fagron	Cloridrato de fenilefrina	14H13-02-309892	1
Fagron	Cloridrato de fenilefrina	14H13-B02	1
Fagron	Cloridrato de fenilefrina	14H13-B02-299814	1
Fagron	Cloridrato de fenilefrina	14H13-B02-299816	2
Fagron	Cloridrato de fenilefrina	14H13B02299817	1
Fagron	Cloridrato de fenilefrina	14H13B02-299817	1
Fagron	Cloridrato de fenilefrina	14H13B02309892	1
Fagron	Cloridrato de fenilefrina	14H13-B02-309892	4
Fagron	Cloridrato de fenilefrina	15F09-B08-316796	2
Fagron	Cloridrato de fenilefrina	16A20-B07-233159	1
Fagron	Cloridrato de fenilefrina	16A20-B07-317987	2
Fagron	Cloridrato de fenilefrina	16A20B07322159	1
Fagron	Cloridrato de fenilefrina	16A20-B07-323398	3
Fagron	Cloridrato de fenilefrina	16A-B07-317987	1
Fagron	Cloridrato de fenilefrina	17C23-B04-333878	3
Fagron	Cloridrato de fenilefrina	17C23-B04-333879	1
Fagron	Cloridrato de fenilefrina	17c23-b04-333880	1
Fagron	Cloridrato de fenilefrina	17C23-B04-333880	1
Fagron	Cloridrato de fenilefrina	17C23-B04-334819	7
Fagron	Cloridrato de fenilefrina	17H18-B02	1
Fagron	Cloridrato de fenilefrina	17-H18-B02	1
Fagron	Cloridrato de fenilefrina	17H18-B02-345401	3
Fagron	Cloridrato de fenilefrina	17H18-B02-348065	1
Fagron	Cloridrato de fenilefrina	17H18-B02-349261	2
Fagron	Cloridrato de fenilefrina	17H18-B02-349262	4
Fagron	Cloridrato de fenilefrina	17H18-B02-353092	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de fenilefrina	17H-18-B02-353092	1
Fagron	Cloridrato de fenilefrina	17-H18-B02-353092	1
Fagron	Cloridrato de fenilefrina	17H18-B02-353093	1
Fagron	Cloridrato de fenilefrina	18L06-B02	8
Fagron	Cloridrato de fenilefrina	18L06-B02-360768	15
Fagron	Cloridrato de fenilefrina	18L06-B02-363037	2
Fagron	Cloridrato de fenilefrina	18L06-B02-367069	4
Fagron	Cloridrato de fenilefrina	18L06-B02-367673	11
Fagron	Cloridrato de fenilefrina	198099-0004	1
Fagron	Cloridrato de fenilefrina	19L06-B02-360768	1
Fagron	Cloridrato de fenilefrina	19L06-B02-367069	1
Fagron	Cloridrato de fenilefrina	20D01-F06	4
Fagron	Cloridrato de fenilefrina	20D01-F06-0003	1
Fagron	Cloridrato de fenilefrina	20D01-F06-370691	8
Fagron	Cloridrato de fenilefrina	20D01-F06-370692	1
Fagron	Cloridrato de fenilefrina	20D01-F06-373487	7
Fagron	Cloridrato de fenilefrina	20G10-F09	2
Fagron	Cloridrato de fenilefrina	20G10-F09-373759	1
Fagron	Cloridrato de fenilefrina	21C04-F02	1
Fagron	Cloridrato de fenilefrina	21C04-F02-377267	1
Fagron	Cloridrato de fenilefrina	21F15-B10	2
Fagron	Cloridrato de fenilefrina	21F15-B10-216432	1
Fagron	Cloridrato de fenilefrina	21F15-B10-217523	6
Fagron	Cloridrato de fenilefrina	2-IL-D-0080117	1
Fagron	Cloridrato de fenilefrina	B02-3670609	1
Fagron	Cloridrato de fenilefrina	B02-3676703	2
Fagron	Cloridrato de fenilefrina	F06-3706900	2
Fagron	Cloridrato de fenilefrina	F06-3706901	2
Fagron	Cloridrato de fenilefrina	F06-3706902	1
Fagron	Cloridrato de fenilefrina	PEH-170717	3
Fagron	Cloridrato de fenilefrina	PEH-200305	1
Gatt-Koller	Cloridrato de fenilefrina	330010164116	1
GEHE	Cloridrato de fenilefrina	17H18-B02	6
GEHE	Cloridrato de fenilefrina	17H18-B02-345401	2
GEHE	Cloridrato de fenilefrina	18L06-B02	3
Jenne	Cloridrato de fenilefrina	14H13-B02	2
JENNE	Cloridrato de fenilefrina	17H18-B02-339756	1
Nachprüfung	Cloridrato de fenilefrina	123456	1
Noweda/Fargon	Cloridrato de fenilefrina	17C23-B04-336301	4
Phoenix	Cloridrato de fenilefrina	15F09-B08	1
PHÖNIX	Cloridrato de fenilefrina	17C23-B04-334819	1

- 235 859 spectra from 1515 *Apo-Ident* customers from a total of 49 169 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de fenilefrina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de fenilefrina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	350	0	152 612
Type B	0	250	0	201 834
Type C	0	208	0	235 859

The substance/substance group *Cloridrato de fenilefrina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2857 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.1154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21051	21960	5,12	299,50
21960	21960	0,00	299,90
22388	22388	0,00	300,33
23394	23394	0,00	298,06
25102	25102	0,00	302,86
25366	21960	5,75	301,39
25823	25823	0,00	291,47
26039	26039	0,00	288,00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de hidromorfona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20296-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de hidromorfona; Hidromorfona, cloridrat; Hydromorphoni hydrochloridum

Special notes

When selecting the *Cloridrato de hidromorfona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de hidromorfona	5	3	31

Second-stage model

For differentiation of the substance/substance group *Cloridrato de hidromorfona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de hidromorfona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ofloxacino	86,29	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de hidromorfona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de hidromorfona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de hidromorfona	13267702	21166	40	0914A-01334
Caelo	Cloridrato de hidromorfona	13267702	21166SI	60	0914A-01334
Caelo	Cloridrato de hidromorfona	15393602	22404	60	1516J-01334
Caelo	Cloridrato de hidromorfona	15393602	22404SI	60	1516J-01334
Fagron	Cloridrato de hidromorfona	13E16-N02	21168	40	0914B-01334
Fagron	Cloridrato de hidromorfona	13E16-N02	21168SI	60	0914B-01334
Fagron	Cloridrato de hidromorfona	13I25-N05	22427	60	1516I-01334
Fagron	Cloridrato de hidromorfona	13I25-N05	22427SI	60	1516I-01334
Fagron	Cloridrato de hidromorfona	15L08-B08-316877	23482	40	1917Q-01334

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 9 reference samples from the substance/substance group *Cloridrato de hidromorfona*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 482 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 7 reference samples from the substance/substance group *Cloridrato de hidromorfona*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de hidromorfona	16123804	23481	40
Caelo	Cloridrato de hidromorfona	18316002	24653	40
Fagron	Cloridrato de hidromorfona	17F01-B01-337510	24652	40
Caelo	Cloridrato de hidromorfona	16123804	23481SI	40
Caelo	Cloridrato de hidromorfona	18316002	24653SI	40
Fagron	Cloridrato de hidromorfona	15L08-B08-316877	23482SI†	40
Fagron	Cloridrato de hidromorfona	17F01-B01-337510	24652SI	40

- 201 804 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 70 spectra from 28 *Apo-Ident* customers from 32 batches from the substance/substance group *Cloridrato de hidromorfona*.

- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de hidromorfona	21002482008	1
Caelo	Cloridrato de hidromorfona	14210405	1
Caelo	Cloridrato de hidromorfona	15393604	1
Caelo	Cloridrato de hidromorfona	15393605	1
Caelo	Cloridrato de hidromorfona	16123805	3
Caelo	Cloridrato de hidromorfona	1623604	1
Caelo	Cloridrato de hidromorfona	16273602	1
Caelo	Cloridrato de hidromorfona	16273604	2
Caelo	Cloridrato de hidromorfona	16273606	1
Caelo	Cloridrato de hidromorfona	16273607	3
Caelo	Cloridrato de hidromorfona	18188402	1
Caelo	Cloridrato de hidromorfona	18188403	1
Caelo	Cloridrato de hidromorfona	18316002	2
Caesar & Loretz GmbH...	Cloridrato de hidromorfona	18188402	1
Caesar & Loretz GmbH...	Cloridrato de hidromorfona	20004514009	3
Caesar & Loretz GmbH...	Cloridrato de hidromorfona	20004525001	2
Caesar & Loretz GmbH...	Cloridrato de hidromorfona	21002482004	3
Caesar & Loretz GmbH	Cloridrato de hidromorfona	18316005	3
Caesar & Loretz GmbH	Cloridrato de hidromorfona	20004514001	14
Caesar & Loretz GmbH	Cloridrato de hidromorfona	20004514004	2
Caesar & Loretz GmbH	Cloridrato de hidromorfona	20004514008	1
Caesar & Loretz GmbH	Cloridrato de hidromorfona	20004525001	2
Caesar & Loretz GmbH	Cloridrato de hidromorfona	21002482001	8
Fagron	Cloridrato de hidromorfona	12G05-N02	1
Fagron	Cloridrato de hidromorfona	13I27-N05	1
Fagron	Cloridrato de hidromorfona	15L08-B08	1
Fagron	Cloridrato de hidromorfona	15L08-B08-316877	1
Fagron	Cloridrato de hidromorfona	17F01-B01-337510	1
Fagron	Cloridrato de hidromorfona	17F0-B01-337510	2
Fagron	Cloridrato de hidromorfona	18I27-B01	1
Fagron	Cloridrato de hidromorfona	18I27-B01-364198	1
Fagron	Cloridrato de hidromorfona	21F03-F01-379168	1
Fargon - Phoenix	Cloridrato de hidromorfona	17F01-B01-3375510	1
Phönix	Cloridrato de hidromorfona	13E16-No2	1

- 235 997 spectra from 1515 *Apo-Ident* customers from a total of 49 227 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de hidromorfona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de hidromorfona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	280	0	201 804
Type C	0	69	1	235 997

The substance/substance group *Cloridrato de hidromorfona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	98.5714 % (> 94.2857 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21166	21166	0,00	113,33
21168	21168	0,00	110,70
22404	22404	0,00	116,72
22427	22427	0,00	111,37
23482	23482	0,00	110,39

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de isoxsuprina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22640-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de isoxsuprina; Isoxsuprina, cloridrato; Isoxsuprini hydrochloridum

Special notes

When selecting the *Cloridrato de isoxsuprina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de isoxsuprina	7	3	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de isoxsuprina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de isoxsuprina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	107,31	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de isoxsuprina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de isoxsuprina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de isoxsuprina	161770	22640	40	20160818*
Caelo	Cloridrato de isoxsuprina	16177001	22735	40	20160818
Caelo	Cloridrato de isoxsuprina	181078	24252	40	20180719*
Euro OTC	Cloridrato de isoxsuprina	1503008-01	22659	40	20150430
Euro OTC	Cloridrato de isoxsuprina	1905019	24920	40	20191128*
Euro OTC	Cloridrato de isoxsuprina	2006035	25285	40	20200706*
Fagron	Cloridrato de isoxsuprina	22I21-B01-233784	27051	40	20230714
Fagron	Cloridrato de isoxsuprina	22I21-B01-233784	27051SI	20	20230714

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 8 reference samples from the substance/substance group *Cloridrato de isoxsuprina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Cloridrato de isoxsuprina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de isoxsuprina	190117	24547	40
Euro OTC	Cloridrato de isoxsuprina	2106006	25760	50
Fagron	Cloridrato de isoxsuprina	20L09-B12-213682	26322	30
Fagron	Cloridrato de isoxsuprina	20L09-B12-213682	26322SI	20

- 201 944 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de isoxsuprina*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de isoxsuprina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de isoxsuprina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	140	0	201 944
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de isoxsuprina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22640	22640	0,00	198,55
22659	22640	5,22	199,87
22735	22640	4,92	196,12
24252	24252	0,00	201,23
24920	24920	0,00	191,60
25285	25285	0,00	195,27
27051	22640	7,56	197,95

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de lidocaína monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20093-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de lidocaína monoidratado; Lidocaína, cloridrato monoidratado; Lidocaini hydrochloridum monohydricum

Special notes

When selecting the *Cloridrato de lidocaína monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de lidocaína monoidratado	7	14	478

Second-stage model

For differentiation of the substance/substance group *Cloridrato de lidocaína monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de lidocaína monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	104,85	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de lidocaína monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de lidocaína monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de lidocaína m…	12135511	20882	40	AR-15-FG-008867-01
Caelo	Cloridrato de lidocaína m…	172923	23807	40	20171122*
Euro OTC	Cloridrato de lidocaína m…	1403025-02	21613	60	20140516
Euro OTC	Cloridrato de lidocaína m…	1411010	21770	60	20150126*
Euro OTC	Cloridrato de lidocaína m…	1907012	24776	40	20190801*
Euro OTC	Cloridrato de lidocaína m…	2201026	26028	40	20220321*
Fagron	Cloridrato de lidocaína m…	20C18-B02-196984	25446	40	20200324

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Cloridrato de lidocaína monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 17 reference samples from the substance/substance group *Cloridrato de lidocaína monoidratado*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de lidocaína m…	162222	22771	40
Caelo	Cloridrato de lidocaína m…	152995	22772	40
Caelo	Cloridrato de lidocaína m…	172048	23687	40
Caelo	Cloridrato de lidocaína m…	20001694	25626	40
Caelo	Cloridrato de lidocaína m…	21002505	25852	50
Caelo	Cloridrato de lidocaína m…	22003202	26491	40
Caelo	Cloridrato de lidocaína m…	23002422	26945	40
Euro OTC	Cloridrato de lidocaína m…	1606024	22702	40
Euro OTC	Cloridrato de lidocaína m…	1612015	22980	40
Euro OTC	Cloridrato de lidocaína m…	1808031	24326	40
Euro OTC	Cloridrato de lidocaína m…	2101034	25572	40
Euro OTC	Cloridrato de lidocaína m…	2211019	26523	40
Euro OTC	Cloridrato de lidocaína m…	2405011	27339	40
Fagron	Cloridrato de lidocaína m…	22C15-B16-218866	26135	40
Caelo	Cloridrato de lidocaína m…	22003202	26491SI	20
Euro OTC	Cloridrato de lidocaína m…	2201026	26028SI†	10
Fagron	Cloridrato de lidocaína m…	22C15-B16-218866	26135SI	20

- 201 464 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3659 spectra from 1120 *Apo-Ident* customers from 497 batches from the substance/substance group *Cloridrato de lidocaína monoidratado*.
- Among them are spectra of independent samples from 474 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de lidocaína m...		1
	Cloridrato de lidocaína m...	21002505006	2
	Cloridrato de lidocaína m...	21002505007	2
	Cloridrato de lidocaína m...	21002505012	2
	Cloridrato de lidocaína m...	2101034-03	2
	Cloridrato de lidocaína m...	220032004	1
	Cloridrato de lidocaína m...	22003202002	11
	Cloridrato de lidocaína m...	22003202003	10
	Cloridrato de lidocaína m...	22003202004	1
	Cloridrato de lidocaína m...	22003202006	5
	Cloridrato de lidocaína m...	22003202007	3
	Cloridrato de lidocaína m...	2201026-01	4
	Cloridrato de lidocaína m...	2201026-02	12
	Cloridrato de lidocaína m...	22110019-003	1
	Cloridrato de lidocaína m...	22110119-01	1
	Cloridrato de lidocaína m...	221101901	1
	Cloridrato de lidocaína m...	2211019-01	70
	Cloridrato de lidocaína m...	2211019-02	8
	Cloridrato de lidocaína m...	2211019-03	4
	Cloridrato de lidocaína m...	22C15-B16-218866	1
	Cloridrato de lidocaína m...	22C15-B16-220953	1
	Cloridrato de lidocaína m...	23003452004	4
	Cloridrato de lidocaína m...	23D25-B11-230225	1
	Cloridrato de lidocaína m...	2405011-01	1
	Cloridrato de lidocaína m...	245011-02	1
	Cloridrato de lidocaína m...	LDH/121043	2
01.07.14	Cloridrato de lidocaína m...	13343004	1
08597954	Cloridrato de lidocaína m...	1907012-01	1
A.H.D.	Cloridrato de lidocaína m...	1202035-02	1
ACM	Cloridrato de lidocaína m...	KNC0625J17	1
ACM	Cloridrato de lidocaína m...	KNC1247J15	1
AEP	Cloridrato de lidocaína m...	22003202003	1
AHC	Cloridrato de lidocaína m...	2211019-02	1
AHD	Cloridrato de lidocaína m...	1612015-02	1
AHD	Cloridrato de lidocaína m...	17292308	2
AHD	Cloridrato de lidocaína m...	17292311	1
AHD	Cloridrato de lidocaína m...	17292313	1
AHD	Cloridrato de lidocaína m...	18179904	1
AHD	Cloridrato de lidocaína m...	18179910	1
AHD	Cloridrato de lidocaína m...	22003202003	1
AHD	Cloridrato de lidocaína m...	2211019-01	2
AHD	Cloridrato de lidocaína m...	23003452004	1
ALH/EuRho	Cloridrato de lidocaína m...	1612015-01	1
ALH	Cloridrato de lidocaína m...	1606024-01	1
Alliance Healt	Cloridrato de lidocaína m...	LDH/722031	1
Alliance health	Cloridrato de lidocaína m...	14B12-B03-292214	1
Alliance	Cloridrato de lidocaína m...	2101034-03	1
Alliance	Cloridrato de lidocaína m...	2211019-01	6
Allianz	Cloridrato de lidocaína m...	17292308	1
Alte Apotheke	Cloridrato de lidocaína m...	1606024-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Cloridrato de lidocaína m…	1202035-03	1
Anzag	Cloridrato de lidocaína m…	1403025-01	1
Anzag	Cloridrato de lidocaína m…	1411010-01	1
Anzag	Cloridrato de lidocaína m…	14B12-B03-292214	1
Anzag	Cloridrato de lidocaína m…	17204804	2
Anzag	Cloridrato de lidocaína m…	1907012-02	1
Anzag	Cloridrato de lidocaína m…	2101034-03	2
Anzag	Cloridrato de lidocaína m…	23003452002	1
Apoident /Sanacorp	Cloridrato de lidocaína m…	2101034-01	2
Apo-Ident, Phönix, 7…	Cloridrato de lidocaína m…	1612015-01	1
apoident/AHD	Cloridrato de lidocaína m…	1808031-03	1
Apo-ident	Cloridrato de lidocaína m…	2101034-02	1
Apo-ident	Cloridrato de lidocaína m…	2101034-03	1
Apo-ident	Cloridrato de lidocaína m…	2201026-01	1
Audor Pharma	Cloridrato de lidocaína m…	2101034-01	1
Bombastus	Cloridrato de lidocaína m…	15215301	1
Bombastus	Cloridrato de lidocaína m…	1606024-01	6
Bombastus	Cloridrato de lidocaína m…	1612015-02	1
Bombastus	Cloridrato de lidocaína m…	180831-01	1
Caelo	Cloridrato de lidocaína m…		1
Caelo	Cloridrato de lidocaína m…	1017Q-01775	1
Caelo	Cloridrato de lidocaína m…	10320703	1
Caelo	Cloridrato de lidocaína m…	10320704	1
Caelo	Cloridrato de lidocaína m…	10320707	2
Caelo	Cloridrato de lidocaína m…	10320717	1
Caelo	Cloridrato de lidocaína m…	10320719	1
Caelo	Cloridrato de lidocaína m…	11091203	1
Caelo	Cloridrato de lidocaína m…	11302902	2
Caelo	Cloridrato de lidocaína m…	11302904	1
Caelo	Cloridrato de lidocaína m…	11302905	1
Caelo	Cloridrato de lidocaína m…	11302906	3
Caelo	Cloridrato de lidocaína m…	116037	1
Caelo	Cloridrato de lidocaína m…	1202035	1
Caelo	Cloridrato de lidocaína m…	120203501	1
Caelo	Cloridrato de lidocaína m…	1202035-02	5
Caelo	Cloridrato de lidocaína m…	1202035-03	1
Caelo	Cloridrato de lidocaína m…	12021503	1
Caelo	Cloridrato de lidocaína m…	12135503	2
Caelo	Cloridrato de lidocaína m…	12135504	3
Caelo	Cloridrato de lidocaína m…	12135508	5
Caelo	Cloridrato de lidocaína m…	12135509	4
Caelo	Cloridrato de lidocaína m…	12135511	2
Caelo	Cloridrato de lidocaína m…	12176101	8
Caelo	Cloridrato de lidocaína m…	12176102	8
Caelo	Cloridrato de lidocaína m…	12176103	8
Caelo	Cloridrato de lidocaína m…	12176109	2
Caelo	Cloridrato de lidocaína m…	1230817/160602402	1
Caelo	Cloridrato de lidocaína m…	12B23-B03-352117	1
Caelo	Cloridrato de lidocaína m…	13(1808031-01)	1
Caelo	Cloridrato de lidocaína m…	13118802	2
Caelo	Cloridrato de lidocaína m…	13118803	5
Caelo	Cloridrato de lidocaína m…	13118807	6
Caelo	Cloridrato de lidocaína m…	13118808	4
Caelo	Cloridrato de lidocaína m…	13118811	2
Caelo	Cloridrato de lidocaína m…	13118812	3
Caelo	Cloridrato de lidocaína m…	1317I-01775	1
Caelo	Cloridrato de lidocaína m…	13343001	2
Caelo	Cloridrato de lidocaína m…	13343002	3
Caelo	Cloridrato de lidocaína m…	13343003	5
Caelo	Cloridrato de lidocaína m…	13343004	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de lidocaína m...	13343007	12
Caelo	Cloridrato de lidocaína m...	13343008	5
Caelo	Cloridrato de lidocaína m...	13343011	3
Caelo	Cloridrato de lidocaína m...	13343012	17
Caelo	Cloridrato de lidocaína m...	13343014	5
Caelo	Cloridrato de lidocaína m...	13343015	2
Caelo	Cloridrato de lidocaína m...	13343016	2
Caelo	Cloridrato de lidocaína m...	13343017	5
Caelo	Cloridrato de lidocaína m...	13343019	4
Caelo	Cloridrato de lidocaína m...	1403025-02	2
Caelo	Cloridrato de lidocaína m...	1411010-01	2
Caelo	Cloridrato de lidocaína m...	1411010-02	1
Caelo	Cloridrato de lidocaína m...	14110101	1
Caelo	Cloridrato de lidocaína m...	14254001	3
Caelo	Cloridrato de lidocaína m...	14J20-B05-303131	1
Caelo	Cloridrato de lidocaína m...	14J20-B05-303133	1
Caelo	Cloridrato de lidocaína m...	15/17-B01-316805	1
Caelo	Cloridrato de lidocaína m...	1505023-01	6
Caelo	Cloridrato de lidocaína m...	1505023-02	2
Caelo	Cloridrato de lidocaína m...	1505023-03	2
Caelo	Cloridrato de lidocaína m...	1515I-01775	1
Caelo	Cloridrato de lidocaína m...	1517-B01-315828	1
Caelo	Cloridrato de lidocaína m...	1521304	1
Caelo	Cloridrato de lidocaína m...	15215201	3
Caelo	Cloridrato de lidocaína m...	15215301	8
Caelo	Cloridrato de lidocaína m...	15215302	2
Caelo	Cloridrato de lidocaína m...	15215303	2
Caelo	Cloridrato de lidocaína m...	15215304	3
Caelo	Cloridrato de lidocaína m...	15215308	3
Caelo	Cloridrato de lidocaína m...	15215309	3
Caelo	Cloridrato de lidocaína m...	15215310	10
Caelo	Cloridrato de lidocaína m...	15215311	6
Caelo	Cloridrato de lidocaína m...	15215312	7
Caelo	Cloridrato de lidocaína m...	152951602714117	1
Caelo	Cloridrato de lidocaína m...	1529906	1
Caelo	Cloridrato de lidocaína m...	15299502	1
Caelo	Cloridrato de lidocaína m...	15299503	11
Caelo	Cloridrato de lidocaína m...	15299506	6
Caelo	Cloridrato de lidocaína m...	15299509	3
Caelo	Cloridrato de lidocaína m...	15299513	9
Caelo	Cloridrato de lidocaína m...	15299514	10
Caelo	Cloridrato de lidocaína m...	15299516	12
Caelo	Cloridrato de lidocaína m...	15299816	1
Caelo	Cloridrato de lidocaína m...	15117-B01	1
Caelo	Cloridrato de lidocaína m...	1603027-01	1
Caelo	Cloridrato de lidocaína m...	1606024	1
Caelo	Cloridrato de lidocaína m...	160602401	1
Caelo	Cloridrato de lidocaína m...	1606024-01	20
Caelo	Cloridrato de lidocaína m...	1606024-02	5
Caelo	Cloridrato de lidocaína m...	160602403	1
Caelo	Cloridrato de lidocaína m...	1606024-03	3
Caelo	Cloridrato de lidocaína m...	160719LC	1
Caelo	Cloridrato de lidocaína m...	16083001	1
Caelo	Cloridrato de lidocaína m...	16101407	1
Caelo	Cloridrato de lidocaína m...	1612015	1
Caelo	Cloridrato de lidocaína m...	1612015_02	1
Caelo	Cloridrato de lidocaína m...	1612015-01	4
Caelo	Cloridrato de lidocaína m...	1612015-02	8
Caelo	Cloridrato de lidocaína m...	1612015-03	4
Caelo	Cloridrato de lidocaína m...	1612015-04	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de lidocaína m...	1612015-05	1
Caelo	Cloridrato de lidocaína m...	16120515-02	1
Caelo	Cloridrato de lidocaína m...	16222202	2
Caelo	Cloridrato de lidocaína m...	16222203	8
Caelo	Cloridrato de lidocaína m...	16222206	2
Caelo	Cloridrato de lidocaína m...	16222207	8
Caelo	Cloridrato de lidocaína m...	16222208	6
Caelo	Cloridrato de lidocaína m...	16222214	13
Caelo	Cloridrato de lidocaína m...	16222215	1
Caelo	Cloridrato de lidocaína m...	168020-0003	1
Caelo	Cloridrato de lidocaína m...	16C09-B03-322144	1
Caelo	Cloridrato de lidocaína m...	17204803	14
Caelo	Cloridrato de lidocaína m...	17204804	32
Caelo	Cloridrato de lidocaína m...	17204810	3
Caelo	Cloridrato de lidocaína m...	17292301	2
Caelo	Cloridrato de lidocaína m...	17292302	6
Caelo	Cloridrato de lidocaína m...	17292304	27
Caelo	Cloridrato de lidocaína m...	17292304907012-02	1
Caelo	Cloridrato de lidocaína m...	17292305	1
Caelo	Cloridrato de lidocaína m...	17292307	5
Caelo	Cloridrato de lidocaína m...	17292308	9
Caelo	Cloridrato de lidocaína m...	17292310	1
Caelo	Cloridrato de lidocaína m...	17292311	9
Caelo	Cloridrato de lidocaína m...	17292313	8
Caelo	Cloridrato de lidocaína m...	17292316	3
Caelo	Cloridrato de lidocaína m...	1729308	1
Caelo	Cloridrato de lidocaína m...	1729311	1
Caelo	Cloridrato de lidocaína m...	1729313	1
Caelo	Cloridrato de lidocaína m...	1792304	1
Caelo	Cloridrato de lidocaína m...	1792313	1
Caelo	Cloridrato de lidocaína m...	17A16-B07	1
Caelo	Cloridrato de lidocaína m...	18041501	1
Caelo	Cloridrato de lidocaína m...	1808031	1
Caelo	Cloridrato de lidocaína m...	1808031-01	12
Caelo	Cloridrato de lidocaína m...	1808031-02	4
Caelo	Cloridrato de lidocaína m...	1808031-03	1
Caelo	Cloridrato de lidocaína m...	1814U-01775	1
Caelo	Cloridrato de lidocaína m...	18179904	19
Caelo	Cloridrato de lidocaína m...	18179905	4
Caelo	Cloridrato de lidocaína m...	18179906	11
Caelo	Cloridrato de lidocaína m...	18179910	8
Caelo	Cloridrato de lidocaína m...	18179911	11
Caelo	Cloridrato de lidocaína m...	18179912	1
Caelo	Cloridrato de lidocaína m...	18179913	1
Caelo	Cloridrato de lidocaína m...	18179914	5
Caelo	Cloridrato de lidocaína m...	18179915	12
Caelo	Cloridrato de lidocaína m...	18179917	1
Caelo	Cloridrato de lidocaína m...	18179922	2
Caelo	Cloridrato de lidocaína m...	18179922/P-06091922	1
Caelo	Cloridrato de lidocaína m...	18179923	4
Caelo	Cloridrato de lidocaína m...	18179924	10
Caelo	Cloridrato de lidocaína m...	18179924P-200319-12	1
Caelo	Cloridrato de lidocaína m...	1819914	1
Caelo	Cloridrato de lidocaína m...	1879904	1
Caelo	Cloridrato de lidocaína m...	18B23-B03	1
Caelo	Cloridrato de lidocaína m...	18B23-B03-347316	1
Caelo	Cloridrato de lidocaína m...	18B23-B03-355046	1
Caelo	Cloridrato de lidocaína m...	18B23-B03-352117	1
Caelo	Cloridrato de lidocaína m...	1907012-01	4
Caelo	Cloridrato de lidocaína m...	1907012-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de lidocaína m...	1907012-03	1
Caelo	Cloridrato de lidocaína m...	1907012-04	1
Caelo	Cloridrato de lidocaína m...	1912M-01775	1
Caelo	Cloridrato de lidocaína m...	1913103	1
Caelo	Cloridrato de lidocaína m...	191350002	14
Caelo	Cloridrato de lidocaína m...	191350004	2
Caelo	Cloridrato de lidocaína m...	191350005	13
Caelo	Cloridrato de lidocaína m...	191350007	3
Caelo	Cloridrato de lidocaína m...	191350008	2
Caelo	Cloridrato de lidocaína m...	191350010	26
Caelo	Cloridrato de lidocaína m...	19135102	1
Caelo	Cloridrato de lidocaína m...	19135103	38
Caelo	Cloridrato de lidocaína m...	19135104	17
Caelo	Cloridrato de lidocaína m...	20004307001	3
Caelo	Cloridrato de lidocaína m...	20004451001	4
Caelo	Cloridrato de lidocaína m...	20004451002	22
Caelo	Cloridrato de lidocaína m...	20004451004	9
Caelo	Cloridrato de lidocaína m...	20004451008	22
Caelo	Cloridrato de lidocaína m...	2004451002	1
Caelo	Cloridrato de lidocaína m...	2021903	1
Caelo	Cloridrato de lidocaína m...	2051301	1
Caelo	Cloridrato de lidocaína m...	20C18-B02-196984	2
Caelo	Cloridrato de lidocaína m...	210025003	1
Caelo	Cloridrato de lidocaína m...	21002505003	7
Caelo	Cloridrato de lidocaína m...	21002505006	6
Caelo	Cloridrato de lidocaína m...	21002505007	8
Caelo	Cloridrato de lidocaína m...	21002505011	2
Caelo	Cloridrato de lidocaína m...	210025505007	1
Caelo	Cloridrato de lidocaína m...	2101034/03	1
Caelo	Cloridrato de lidocaína m...	2101034-01	1
Caelo	Cloridrato de lidocaína m...	2101034-02	1
Caelo	Cloridrato de lidocaína m...	2101034-03	2
Caelo	Cloridrato de lidocaína m...	21101034-03	1
Caelo	Cloridrato de lidocaína m...	21C05-B05-210126	1
Caelo	Cloridrato de lidocaína m...	22003202002	6
Caelo	Cloridrato de lidocaína m...	22003202003	2
Caelo	Cloridrato de lidocaína m...	2201026-01	1
Caelo	Cloridrato de lidocaína m...	2201026-02	2
Caelo	Cloridrato de lidocaína m...	22042003	1
Caelo	Cloridrato de lidocaína m...	2211019-01	1
Caelo	Cloridrato de lidocaína m...	2211o19-01	1
Caelo	Cloridrato de lidocaína m...	23011403	1
Caelo	Cloridrato de lidocaína m...	24071401	1
Caelo	Cloridrato de lidocaína m...	25091202	1
Caelo	Cloridrato de lidocaína m...	26041401	1
Caelo	Cloridrato de lidocaína m...	26051802	1
Caelo	Cloridrato de lidocaína m...	26071303	1
Caelo	Cloridrato de lidocaína m...	280501	1
Caelo	Cloridrato de lidocaína m...	28111812	1
Caelo	Cloridrato de lidocaína m...	29081503	1
Caelo	Cloridrato de lidocaína m...	3071711	1
Caelo	Cloridrato de lidocaína m...	4051703	1
Caelo	Cloridrato de lidocaína m...	4111302	1
Caelo	Cloridrato de lidocaína m...	4111703	1
Caelo	Cloridrato de lidocaína m...	415299506	1
Caelo	Cloridrato de lidocaína m...	5113E-01775	1
Caelo	Cloridrato de lidocaína m...	5211E-01775	1
Caelo	Cloridrato de lidocaína m...	6121706	1
Caelo	Cloridrato de lidocaína m...	812-16001	1
Caelo	Cloridrato de lidocaína m...	AKD14	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de lidocaína m...	LDH/118024	1
Caerlo	Cloridrato de lidocaína m...	13118807	1
Caesar & Lorenz GmbH	Cloridrato de lidocaína m...	16222208	1
Caesar & Lorenz GmbH	Cloridrato de lidocaína m...	18179923	2
Caesar & Lorenz GmbH	Cloridrato de lidocaína m...	19135104	1
Caesar & Lorenz GmbH	Cloridrato de lidocaína m...	2273185	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	18179915	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	19135103	1
Caesar & Loretz GmbH/ AEP	Cloridrato de lidocaína m...	191350002	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	21002505011	2
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	191350002	1
Caesar & Loretz GmbH/AHD	Cloridrato de lidocaína m...	19135103	2
Caesar & Loretz GmbH/AHD	Cloridrato de lidocaína m...	21002505003	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	21002505006	2
Caesar & Loretz GmbH/Gehe	Cloridrato de lidocaína m...	20004451002	3
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	18179914	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	191350002	2
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	191350010	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	20004451002	2
Caesar & Loretz GmbH/Gö	Cloridrato de lidocaína m...	191350010	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	19135103	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	19135103	2
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	18179914	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	18179917	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	191350010	1
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	20004451002	2
Caesar & Loretz GmbH...	Cloridrato de lidocaína m...	20004451002	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	13343002	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	15215201	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	1612015-03	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	16222203	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	17292311	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179903	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179904	4
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179905	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179906	2
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179911	4
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179912	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179914	4
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179916	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179922	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	18179923	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	1907012-02	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	191350002	7
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	191350004	3
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	191350005	2
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	191350007	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	191350010	10
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	19135103	6
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	19135104	4
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	20004451002	15
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	20004451004	6
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	20004451008	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	210025050004	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	21002505006	2
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	21002505007	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	21002505008	1
Caesar & Loretz GmbH	Cloridrato de lidocaína m...	22003202003	3
Caesar & Loretz/Anza...	Cloridrato de lidocaína m...	18179906	1
Caesar & Loretz	Cloridrato de lidocaína m...	1612015-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar u Loretz	Cloridrato de lidocaína m...	13343017	1
Caesar&Loretz GmbH /Anzag	Cloridrato de lidocaína m...	15215303	1
Caesar&Loretz GmbH/ ...	Cloridrato de lidocaína m...	17204803	1
Caesar&Loretz GmbH/Anzag	Cloridrato de lidocaína m...	13118803	2
Caeser und Loretz GmbH	Cloridrato de lidocaína m...	181799023	1
Caleo/ Noweda	Cloridrato de lidocaína m...	17204804	1
Caolo	Cloridrato de lidocaína m...	13343008	1
Cealo	Cloridrato de lidocaína m...	20004451008	1
Ensbona/ Sanacorp	Cloridrato de lidocaína m...	1606024-01	1
EuRho / Alliance	Cloridrato de lidocaína m...	1907012-03	1
EuRho / Alliance	Cloridrato de lidocaína m...	2101034-01	1
EuRho / Phönix	Cloridrato de lidocaína m...	2201026-01	1
EuRho / Sanacorp	Cloridrato de lidocaína m...	1907012-04	1
EuRho/ Anzag	Cloridrato de lidocaína m...	2201026-01	3
EuRho/ Jenne	Cloridrato de lidocaína m...	2101034-02	1
Eurho/ Noweda	Cloridrato de lidocaína m...	1808031-01	1
Eurho/ Noweda	Cloridrato de lidocaína m...	1808031-03	2
EuRho/ Phönix	Cloridrato de lidocaína m...	1612015-04	1
EuRho/ Sana	Cloridrato de lidocaína m...	1808031-02	1
EuRho/ VDL	Cloridrato de lidocaína m...	1612015-04	1
EuRho/AHD	Cloridrato de lidocaína m...	1907012-01	1
EuRho/AHD	Cloridrato de lidocaína m...	LDH/720023	2
EuRho/Gehe	Cloridrato de lidocaína m...	2101034-01	3
EuRho/Jenne	Cloridrato de lidocaína m...	1907012-02	1
Eurho/Jenne	Cloridrato de lidocaína m...	1907012-04	1
EuRho/Jenne	Cloridrato de lidocaína m...	2101034-03	1
EuRho/Noweda	Cloridrato de lidocaína m...	1612015-02	2
EuRho/Noweda	Cloridrato de lidocaína m...	2101034-01	1
EuRho/Phoenix	Cloridrato de lidocaína m...	1612015-01	1
EuRho/Phoenix	Cloridrato de lidocaína m...	2201026-02	1
EuRho/Phönix	Cloridrato de lidocaína m...	1808031-01	2
EuRho/Phönix	Cloridrato de lidocaína m...	2101034-01	1
EuRho/Sanacorp	Cloridrato de lidocaína m...	1612015-04	1
EuRho/Sanacorp	Cloridrato de lidocaína m...	1808031-01	3
EuRho/VDL	Cloridrato de lidocaína m...	1612015-03	2
EuRho	Cloridrato de lidocaína m...	1108017-01	3
EuRho	Cloridrato de lidocaína m...	140302501	1
EuRho	Cloridrato de lidocaína m...	1403025-02	1
EuRho	Cloridrato de lidocaína m...	1505023-01	4
EuRho	Cloridrato de lidocaína m...	1505023-02	1
EuRho	Cloridrato de lidocaína m...	1612015-01	2
EuRho	Cloridrato de lidocaína m...	161201502	1
EuRho	Cloridrato de lidocaína m...	1612015-02	1
EuRho	Cloridrato de lidocaína m...	1612015-04	1
EuRho	Cloridrato de lidocaína m...	18008031	1
EuRho	Cloridrato de lidocaína m...	1808031-02	2
EuRho	Cloridrato de lidocaína m...	1808031-03	1
Eurho	Cloridrato de lidocaína m...	1907012-02	1
EuRho	Cloridrato de lidocaína m...	2101034	1
Eurho	Cloridrato de lidocaína m...	2101034-01	1
EuRho	Cloridrato de lidocaína m...	2101034-03	1
Eurho	Cloridrato de lidocaína m...	2101034-04	1
EuRho	Cloridrato de lidocaína m...	2201026-01	1
EuRho	Cloridrato de lidocaína m...	2201026-02	2
EuRho	Cloridrato de lidocaína m...	2211019-01	1
EuRho	Cloridrato de lidocaína m...	EuRho	1
EuRho	Cloridrato de lidocaína m...	LDH720023	1
Euro OTC	Cloridrato de lidocaína m...		4
Euro OTC	Cloridrato de lidocaína m...	1004040-01	1
Euro OTC	Cloridrato de lidocaína m...	1010024-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de lidocaína m...	1066024-01	1
Euro OTC	Cloridrato de lidocaína m...	1103034-01	2
Euro OTC	Cloridrato de lidocaína m...	1108017-01	5
Euro OTC	Cloridrato de lidocaína m...	1108017-02	7
Euro OTC	Cloridrato de lidocaína m...	1140917/160602403	1
Euro OTC	Cloridrato de lidocaína m...	1202034-01	2
Euro OTC	Cloridrato de lidocaína m...	1202035	1
Euro OTC	Cloridrato de lidocaína m...	1202035/02	1
Euro OTC	Cloridrato de lidocaína m...	1202035-01	24
Euro OTC	Cloridrato de lidocaína m...	120203502	3
Euro OTC	Cloridrato de lidocaína m...	1202035-02	35
Euro OTC	Cloridrato de lidocaína m...	1202035-03	11
Euro OTC	Cloridrato de lidocaína m...	1202035-1	1
Euro OTC	Cloridrato de lidocaína m...	12020351612015-01	1
Euro OTC	Cloridrato de lidocaína m...	1401010-01	1
Euro OTC	Cloridrato de lidocaína m...	1403025	1
Euro OTC	Cloridrato de lidocaína m...	140302501	2
Euro OTC	Cloridrato de lidocaína m...	1403025-01	22
Euro OTC	Cloridrato de lidocaína m...	140302502	2
Euro OTC	Cloridrato de lidocaína m...	1403025-02	15
Euro OTC	Cloridrato de lidocaína m...	1403025-03	1
Euro OTC	Cloridrato de lidocaína m...	140415A	1
Euro OTC	Cloridrato de lidocaína m...	141101	1
Euro OTC	Cloridrato de lidocaína m...	141101001	4
Euro OTC	Cloridrato de lidocaína m...	1411010-01	39
Euro OTC	Cloridrato de lidocaína m...	1411010-01Mg25g	1
Euro OTC	Cloridrato de lidocaína m...	141101002	3
Euro OTC	Cloridrato de lidocaína m...	1411010-02	26
Euro OTC	Cloridrato de lidocaína m...	1411010-02Mg50g	1
Euro OTC	Cloridrato de lidocaína m...	141101-01	1
Euro OTC	Cloridrato de lidocaína m...	14110101-01	1
Euro OTC	Cloridrato de lidocaína m...	1411010-2	1
Euro OTC	Cloridrato de lidocaína m...	150502301	3
Euro OTC	Cloridrato de lidocaína m...	1505023-01	71
Euro OTC	Cloridrato de lidocaína m...	1505023-02	21
Euro OTC	Cloridrato de lidocaína m...	1505023-03	16
Euro OTC	Cloridrato de lidocaína m...	150523-02	1
Euro OTC	Cloridrato de lidocaína m...	1512015-04	1
Euro OTC	Cloridrato de lidocaína m...	1600024-02	1
Euro OTC	Cloridrato de lidocaína m...	16006024-02	1
Euro OTC	Cloridrato de lidocaína m...	1606021-01	1
Euro OTC	Cloridrato de lidocaína m...	1606024_02	3
Euro OTC	Cloridrato de lidocaína m...	160602401	3
Euro OTC	Cloridrato de lidocaína m...	1606024-01	67
Euro OTC	Cloridrato de lidocaína m...	160602402	2
Euro OTC	Cloridrato de lidocaína m...	1606024-02	76
Euro OTC	Cloridrato de lidocaína m...	1606024-03	24
Euro OTC	Cloridrato de lidocaína m...	1606024-1	1
Euro OTC	Cloridrato de lidocaína m...	160624-01	1
Euro OTC	Cloridrato de lidocaína m...	16112015-01	2
Euro OTC	Cloridrato de lidocaína m...	16112015-04	1
Euro OTC	Cloridrato de lidocaína m...	1612012015-04	1
Euro OTC	Cloridrato de lidocaína m...	1612015	6
Euro OTC	Cloridrato de lidocaína m...	1612015_01	1
Euro OTC	Cloridrato de lidocaína m...	161201501	1
Euro OTC	Cloridrato de lidocaína m...	1612015-01	51
Euro OTC	Cloridrato de lidocaína m...	161201502	3
Euro OTC	Cloridrato de lidocaína m...	1612015-02	74
Euro OTC	Cloridrato de lidocaína m...	1612015-03	24
Euro OTC	Cloridrato de lidocaína m...	161201504	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de lidocaína m...	1612015-04	36
Euro OTC	Cloridrato de lidocaína m...	1612015-05	3
Euro OTC	Cloridrato de lidocaína m...	1612015-14	1
Euro OTC	Cloridrato de lidocaína m...	16122016-01	1
Euro OTC	Cloridrato de lidocaína m...	1618015-02	1
Euro OTC	Cloridrato de lidocaína m...	168020	2
Euro OTC	Cloridrato de lidocaína m...	170612182	1
Euro OTC	Cloridrato de lidocaína m...	171106LHC/1606024-03	1
Euro OTC	Cloridrato de lidocaína m...	17204803	2
Euro OTC	Cloridrato de lidocaína m...	17204810	1
Euro OTC	Cloridrato de lidocaína m...	180220L/1612015-01	1
Euro OTC	Cloridrato de lidocaína m...	18080031	1
Euro OTC	Cloridrato de lidocaína m...	180803-01	1
Euro OTC	Cloridrato de lidocaína m...	1808031	5
Euro OTC	Cloridrato de lidocaína m...	180803101	4
Euro OTC	Cloridrato de lidocaína m...	1808031-01	119
Euro OTC	Cloridrato de lidocaína m...	1808031-01Retest	1
Euro OTC	Cloridrato de lidocaína m...	180803102	2
Euro OTC	Cloridrato de lidocaína m...	1808031-02	88
Euro OTC	Cloridrato de lidocaína m...	180803103	1
Euro OTC	Cloridrato de lidocaína m...	1808031-03	40
Euro OTC	Cloridrato de lidocaína m...	1808031-04	1
Euro OTC	Cloridrato de lidocaína m...	18908031-01	1
Euro OTC	Cloridrato de lidocaína m...	1907012	2
Euro OTC	Cloridrato de lidocaína m...	1907012_01	1
Euro OTC	Cloridrato de lidocaína m...	190701201	4
Euro OTC	Cloridrato de lidocaína m...	1907012-01	151
Euro OTC	Cloridrato de lidocaína m...	190701202	1
Euro OTC	Cloridrato de lidocaína m...	1907012-02	110
Euro OTC	Cloridrato de lidocaína m...	1907012-03	91
Euro OTC	Cloridrato de lidocaína m...	190701204	1
Euro OTC	Cloridrato de lidocaína m...	1907012-04	62
Euro OTC	Cloridrato de lidocaína m...	1907012-1	3
Euro OTC	Cloridrato de lidocaína m...	1907012-12	1
Euro OTC	Cloridrato de lidocaína m...	1907012-42	1
Euro OTC	Cloridrato de lidocaína m...	1907012-62	1
Euro OTC	Cloridrato de lidocaína m...	1907013-03	1
Euro OTC	Cloridrato de lidocaína m...	190720107	1
Euro OTC	Cloridrato de lidocaína m...	19097012-01	1
Euro OTC	Cloridrato de lidocaína m...	197012-09	1
Euro OTC	Cloridrato de lidocaína m...	20131010-4	1
Euro OTC	Cloridrato de lidocaína m...	20C18-B02-196984	1
Euro OTC	Cloridrato de lidocaína m...	210034-02	1
Euro OTC	Cloridrato de lidocaína m...	2101031-01	1
Euro OTC	Cloridrato de lidocaína m...	2101034	1
Euro OTC	Cloridrato de lidocaína m...	210103401	1
Euro OTC	Cloridrato de lidocaína m...	2101034-01	57
Euro OTC	Cloridrato de lidocaína m...	2101034-02	46
Euro OTC	Cloridrato de lidocaína m...	210103403	1
Euro OTC	Cloridrato de lidocaína m...	2101034-03	38
Euro OTC	Cloridrato de lidocaína m...	2101034-04	7
Euro OTC	Cloridrato de lidocaína m...	2101034-3	1
Euro OTC	Cloridrato de lidocaína m...	2201026	2
Euro OTC	Cloridrato de lidocaína m...	2201026_01	1
Euro OTC	Cloridrato de lidocaína m...	220102601	4
Euro OTC	Cloridrato de lidocaína m...	2201026-01	102
Euro OTC	Cloridrato de lidocaína m...	2201026-02	44
Euro OTC	Cloridrato de lidocaína m...	2201026-1	1
Euro OTC	Cloridrato de lidocaína m...	2201062-01	1
Euro OTC	Cloridrato de lidocaína m...	220126-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de lidocaína m...	22101901	1
Euro OTC	Cloridrato de lidocaína m...	221019-01	2
Euro OTC	Cloridrato de lidocaína m...	221026-02	1
Euro OTC	Cloridrato de lidocaína m...	221101901	2
Euro OTC	Cloridrato de lidocaína m...	2211019-01	13
Euro OTC	Cloridrato de lidocaína m...	2213U01775	1
Euro OTC	Cloridrato de lidocaína m...	230816O1	1
Euro OTC	Cloridrato de lidocaína m...	2805016-01	1
Euro OTC	Cloridrato de lidocaína m...	2810029-01	1
Euro OTC	Cloridrato de lidocaína m...	2886	1
Euro OTC	Cloridrato de lidocaína m...	991011	1
Euro OTC	Cloridrato de lidocaína m...	AP220802-02	1
Euro OTC	Cloridrato de lidocaína m...	ldh/116023	1
Euro OTC	Cloridrato de lidocaína m...	LDH/116023	3
Euro OTC	Cloridrato de lidocaína m...	LDH/118024	4
Euro OTC	Cloridrato de lidocaína m...	LDH/121043	4
Euro OTC	Cloridrato de lidocaína m...	LDH/719007	5
Euro OTC	Cloridrato de lidocaína m...	LDH/720023	2
Euro OTC	Cloridrato de lidocaína m...	LDH/722031	1
Euro OTC	Cloridrato de lidocaína m...	LDHI719007	1
Euro OTC	Cloridrato de lidocaína m...	LDHV121043	1
Euro OTC	Cloridrato de lidocaína m...	lhd719007	1
Euro OTC	Cloridrato de lidocaína m...	LID-20-11-001	2
Euro/ Anzag	Cloridrato de lidocaína m...	1606024-03	1
Euro/ Gehe	Cloridrato de lidocaína m...	1808031-03	1
Euro/ Gehe	Cloridrato de lidocaína m...	1907012-01	2
Euro/ Gehe	Cloridrato de lidocaína m...	1907012-02	1
Euro/ Jenne	Cloridrato de lidocaína m...	1907012-02	1
Euro/Alliance Healthcare	Cloridrato de lidocaína m...	150523-01	1
euro/Gehe	Cloridrato de lidocaína m...	1907012-04	1
Euro/Gehe	Cloridrato de lidocaína m...	2201026-02	1
Euro/Phoenix	Cloridrato de lidocaína m...	1907012-01	3
Euro/Phönix	Cloridrato de lidocaína m...	141101010-01	1
Euro/Phönix	Cloridrato de lidocaína m...	1612015-01	1
Euro/Phönix	Cloridrato de lidocaína m...	1808031-02	1
Euro/Phönix	Cloridrato de lidocaína m...	1808031-03	1
Euro/Phönix	Cloridrato de lidocaína m...	210103401	1
Euro/Phönix	Cloridrato de lidocaína m...	2101034-03	1
Euro/Sanacorp	Cloridrato de lidocaína m...	1808031-03	1
Euro/Sanacorp	Cloridrato de lidocaína m...	2101034-01	1
Euro	Cloridrato de lidocaína m...	1505023-01	2
Europ Ots Pharma	Cloridrato de lidocaína m...	1403025-01	1
EuroPharm	Cloridrato de lidocaína m...	1907012-02	1
Europharm	Cloridrato de lidocaína m...	2101034-02	4
EuroPharm	Cloridrato de lidocaína m...	2101034-02	1
Fagon	Cloridrato de lidocaína m...	15/17-B01-316805	1
Fagron	Cloridrato de lidocaína m...	11H18-N01	1
Fagron	Cloridrato de lidocaína m...	11L09-N09	2
Fagron	Cloridrato de lidocaína m...	1202035-02	1
Fagron	Cloridrato de lidocaína m...	12c05-N02	1
Fagron	Cloridrato de lidocaína m...	12C05-N02	1
Fagron	Cloridrato de lidocaína m...	12E14-N04	2
Fagron	Cloridrato de lidocaína m...	12H09-N08	2
Fagron	Cloridrato de lidocaína m...	13218-B11	1
Fagron	Cloridrato de lidocaína m...	13F07N06	1
Fagron	Cloridrato de lidocaína m...	13F07-N06	7
Fagron	Cloridrato de lidocaína m...	13L18-B11-286901	1
Fagron	Cloridrato de lidocaína m...	14/20-B05	1
Fagron	Cloridrato de lidocaína m...	1420-b05-303	1
Fagron	Cloridrato de lidocaína m...	14B12-B03-292214	9

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de lidocaína m...	14e13-b06-294973	1
Fagron	Cloridrato de lidocaína m...	14e13-b06-294975	2
Fagron	Cloridrato de lidocaína m...	14E13-B06-294975	5
Fagron	Cloridrato de lidocaína m...	14J07-B04-299433	4
Fagron	Cloridrato de lidocaína m...	14J07-B04-299434	2
Fagron	Cloridrato de lidocaína m...	14J20-b05	1
Fagron	Cloridrato de lidocaína m...	14J20-B05-303131	2
Fagron	Cloridrato de lidocaína m...	14j20-b05-303133	1
Fagron	Cloridrato de lidocaína m...	14J20-B05-303133	2
Fagron	Cloridrato de lidocaína m...	15/17-b01-315828	1
Fagron	Cloridrato de lidocaína m...	15/17-B01316805	1
Fagron	Cloridrato de lidocaína m...	15/17-B01-316805	8
Fagron	Cloridrato de lidocaína m...	1505023-01	2
Fagron	Cloridrato de lidocaína m...	1517-801	1
Fagron	Cloridrato de lidocaína m...	1517-B01	1
Fagron	Cloridrato de lidocaína m...	15215311	2
Fagron	Cloridrato de lidocaína m...	15299513	1
Fagron	Cloridrato de lidocaína m...	15299516	1
Fagron	Cloridrato de lidocaína m...	15I17-B01-315828	2
Fagron	Cloridrato de lidocaína m...	15I17-b01-316805	1
Fagron	Cloridrato de lidocaína m...	15I17-B01-316805	2
Fagron	Cloridrato de lidocaína m...	161201501	1
Fagron	Cloridrato de lidocaína m...	1612015-01	1
Fagron	Cloridrato de lidocaína m...	1612015-02	3
Fagron	Cloridrato de lidocaína m...	1612015-03	1
Fagron	Cloridrato de lidocaína m...	168020-0001	1
Fagron	Cloridrato de lidocaína m...	16C09-B03	1
Fagron	Cloridrato de lidocaína m...	16C09-B03-319230	1
Fagron	Cloridrato de lidocaína m...	16c09b03322144	1
Fagron	Cloridrato de lidocaína m...	16C09-B03-322144	4
Fagron	Cloridrato de lidocaína m...	16c09-b03-322145	2
Fagron	Cloridrato de lidocaína m...	16C09-B03-322145	1
Fagron	Cloridrato de lidocaína m...	16J24-B15-329421	1
Fagron	Cloridrato de lidocaína m...	17A16-B07	2
Fagron	Cloridrato de lidocaína m...	17A16-B07-331959	4
Fagron	Cloridrato de lidocaína m...	17A16B07333010	1
Fagron	Cloridrato de lidocaína m...	17A16-B07-333010	4
Fagron	Cloridrato de lidocaína m...	17G10-B08-342287	1
Fagron	Cloridrato de lidocaína m...	17G10-B08-346659	3
Fagron	Cloridrato de lidocaína m...	17G10-B08-346659	1
Fagron	Cloridrato de lidocaína m...	1808031-01	1
Fagron	Cloridrato de lidocaína m...	1808031-02	2
Fagron	Cloridrato de lidocaína m...	1808031-03	1
Fagron	Cloridrato de lidocaína m...	18B23-B03	5
Fagron	Cloridrato de lidocaína m...	18B23-B03_355046	1
Fagron	Cloridrato de lidocaína m...	18B23-B03-347316	5
Fagron	Cloridrato de lidocaína m...	18B23-B03-348590	3
Fagron	Cloridrato de lidocaína m...	18B23-B03-348748	1
Fagron	Cloridrato de lidocaína m...	18B23-B03-352117	4
Fagron	Cloridrato de lidocaína m...	18B23-B03-353035	1
Fagron	Cloridrato de lidocaína m...	18B23-B03-354288	5
Fagron	Cloridrato de lidocaína m...	18B23-B03-355046	1
Fagron	Cloridrato de lidocaína m...	18B23-B03-355381	1
Fagron	Cloridrato de lidocaína m...	18B23-B04-348590	1
Fagron	Cloridrato de lidocaína m...	1907012-02	1
Fagron	Cloridrato de lidocaína m...	19E22-B01-1914608	1
Fagron	Cloridrato de lidocaína m...	19E22-B01-191467	5
Fagron	Cloridrato de lidocaína m...	19E22-B01-191468	9
Fagron	Cloridrato de lidocaína m...	19J16-B02	1
Fagron	Cloridrato de lidocaína m...	19J16-B02-196983	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de lidocaína m...	19j16-b02-196985	1
Fagron	Cloridrato de lidocaína m...	19J16-B02-196993	2
Fagron	Cloridrato de lidocaína m...	19J16-BO2-196983	2
Fagron	Cloridrato de lidocaína m...	20A31-B06	2
Fagron	Cloridrato de lidocaína m...	20A31-B06-196986	1
Fagron	Cloridrato de lidocaína m...	20A31-B06-2005105	1
Fagron	Cloridrato de lidocaína m...	20A31-B06-200515	6
Fagron	Cloridrato de lidocaína m...	20C18B02	1
Fagron	Cloridrato de lidocaína m...	20C18-B02	1
Fagron	Cloridrato de lidocaína m...	20c18-b02-196984	1
Fagron	Cloridrato de lidocaína m...	20C18-B02-196984	9
Fagron	Cloridrato de lidocaína m...	20E28-B04-201210	1
Fagron	Cloridrato de lidocaína m...	20e28-b04-201268	1
Fagron	Cloridrato de lidocaína m...	20E28-B04-201302	1
Fagron	Cloridrato de lidocaína m...	20E28-B04-201702	3
Fagron	Cloridrato de lidocaína m...	20E28-B04-2017021	1
Fagron	Cloridrato de lidocaína m...	21/17-803-216827	1
Fagron	Cloridrato de lidocaína m...	21/17-B03-216798	2
Fagron	Cloridrato de lidocaína m...	21/17-B03-216827	1
Fagron	Cloridrato de lidocaína m...	218I-01775	1
Fagron	Cloridrato de lidocaína m...	21A12B04203052	1
Fagron	Cloridrato de lidocaína m...	21A12-B04-203052	2
Fagron	Cloridrato de lidocaína m...	21C05-B05-210126	1
Fagron	Cloridrato de lidocaína m...	21I17-B03	1
Fagron	Cloridrato de lidocaína m...	21I17-B03-213766	2
Fagron	Cloridrato de lidocaína m...	21I17-B03-213769	4
Fagron	Cloridrato de lidocaína m...	21I17-B03-216798	1
Fagron	Cloridrato de lidocaína m...	21I17-BO3	1
Fagron	Cloridrato de lidocaína m...	21l17-B03-213769	1
Fagron	Cloridrato de lidocaína m...	2201026-01	1
Fagron	Cloridrato de lidocaína m...	22C15-B16	1
Fagron	Cloridrato de lidocaína m...	22C15-B16-218866	1
Fagron	Cloridrato de lidocaína m...	22C15-B16-220955	2
Fagron	Cloridrato de lidocaína m...	22H22-B03-224257	1
Fagron	Cloridrato de lidocaína m...	4612Q-01775	1
Fagron	Cloridrato de lidocaína m...	812-16001	3
Fagron	Cloridrato de lidocaína m...	8F26-N07	1
Fagron	Cloridrato de lidocaína m...	9B3M1L2Fo118	1
Fagron	Cloridrato de lidocaína m...	9E08-N03	1
Fagron	Cloridrato de lidocaína m...	B01-1914608	1
Fagron	Cloridrato de lidocaína m...	B02-1969803	1
Fagron	Cloridrato de lidocaína m...	B02-1969804	3
Fagron	Cloridrato de lidocaína m...	B03-2167908	1
Fagron	Cloridrato de lidocaína m...	B04-2030502	2
Fagron	Cloridrato de lidocaína m...	LDH/116023	1
Fagron	Cloridrato de lidocaína m...	LDH/116037	2
Fagron	Cloridrato de lidocaína m...	LDH/117022	1
Fagron	Cloridrato de lidocaína m...	LDH/117049	1
Fagron	Cloridrato de lidocaína m...	LDH/118024	1
Fagron	Cloridrato de lidocaína m...	LDH/119022	1
Fagron	Cloridrato de lidocaína m...	LDH-721013	1
Fargon GmbH & Co.KG	Cloridrato de lidocaína m...	15/17-B01-316805	1
Fargon GmbH & Co.KG	Cloridrato de lidocaína m...	16C09-B03-322144	2
Fargon	Cloridrato de lidocaína m...	20C18-B02-196948	1
fargon	Cloridrato de lidocaína m...	720005	1
Fiebig 04.7.13 EK 4,54	Cloridrato de lidocaína m...	12135511	1
Fiebig	Cloridrato de lidocaína m...	1808031-01	1
Fiebig	Cloridrato de lidocaína m...	1907012-01	1
Fiebig	Cloridrato de lidocaína m...	20C18-B02-196984	1
Finze	Cloridrato de lidocaína m...	1202035-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Frago/Noweda	Cloridrato de lidocaína m...	6108-05-0	1
Gatt-Koller	Cloridrato de lidocaína m...	1801084	1
Gehe amax	Cloridrato de lidocaína m...	17292308	1
Gehe amax	Cloridrato de lidocaína m...	19135103	1
Gehe Rostock	Cloridrato de lidocaína m...	2201026-01	1
Gehe/EuRho	Cloridrato de lidocaína m...	1907012-02	1
Gehe/Euro	Cloridrato de lidocaína m...	1612015-02	1
Gehe	Cloridrato de lidocaína m...	1190313	1
Gehe	Cloridrato de lidocaína m...	1202035-02	1
Gehe	Cloridrato de lidocaína m...	12C05-N02	2
Gehe	Cloridrato de lidocaína m...	1411010-01	1
Gehe	Cloridrato de lidocaína m...	141101002	1
Gehe	Cloridrato de lidocaína m...	15215304	1
Gehe	Cloridrato de lidocaína m...	15299513	1
Gehe	Cloridrato de lidocaína m...	15299516	1
Gehe	Cloridrato de lidocaína m...	1606024-02	1
GEHE	Cloridrato de lidocaína m...	1606024-02	1
Gehe	Cloridrato de lidocaína m...	1612015-01	1
GEHE	Cloridrato de lidocaína m...	1612015-01	1
Gehe	Cloridrato de lidocaína m...	1612015-02	2
GEHE	Cloridrato de lidocaína m...	1612015-02	1
Gehe	Cloridrato de lidocaína m...	16222207	1
GEHE	Cloridrato de lidocaína m...	16222214	1
GEHE	Cloridrato de lidocaína m...	17292312	1
Gehe	Cloridrato de lidocaína m...	1808031-01	1
Gehe	Cloridrato de lidocaína m...	1808031-02	1
Gehe	Cloridrato de lidocaína m...	18179904	1
Gehe	Cloridrato de lidocaína m...	1907012-01	5
Gehe	Cloridrato de lidocaína m...	1907012-02	2
Gehe	Cloridrato de lidocaína m...	1907012-03	1
Gehe	Cloridrato de lidocaína m...	191350002	2
Gehe	Cloridrato de lidocaína m...	191350007	1
Gehe	Cloridrato de lidocaína m...	2101034-01	1
Gehe	Cloridrato de lidocaína m...	2201026-01	1
Gehe	Cloridrato de lidocaína m...	2201026-02	4
Gehe	Cloridrato de lidocaína m...	221026-01	1
Gehe	Cloridrato de lidocaína m...	2211019-01	4
Gehe	Cloridrato de lidocaína m...	23003452004	1
Gehe	Cloridrato de lidocaína m...	LDH/116023	1
Gehe	Cloridrato de lidocaína m...	LDH/719007	1
Geibo/EuRho	Cloridrato de lidocaína m...	1515023-01	1
Geibo/Euro 29.8.	Cloridrato de lidocaína m...	1808031-02	1
GMP Konform	Cloridrato de lidocaína m...	20A31-B06	1
Hänseler	Cloridrato de lidocaína m...		3
Hedinger/Ebert	Cloridrato de lidocaína m...	13118807	1
INTERN-DROGEN	Cloridrato de lidocaína m...	20004451008	1
INTERN-DROGEN	Cloridrato de lidocaína m...	21002505006	1
Jenne	Cloridrato de lidocaína m...	1808031-02	1
Jenne	Cloridrato de lidocaína m...	1907012-04	1
Jenne	Cloridrato de lidocaína m...	2101034-02	1
Kehr/EuRho	Cloridrato de lidocaína m...	1907012-03	1
Kehr	Cloridrato de lidocaína m...	1606024-02	1
Kehr	Cloridrato de lidocaína m...	1612015-01	1
Kehr	Cloridrato de lidocaína m...	1612015-02	1
Kehr	Cloridrato de lidocaína m...	1612015-03	1
Kehr	Cloridrato de lidocaína m...	21002505007	1
Kehr	Cloridrato de lidocaína m...	22003202003	1
Kehr	Cloridrato de lidocaína m...	22003202007	1
Klenk	Cloridrato de lidocaína m...	1612015-01	2
kögl	Cloridrato de lidocaína m...	1803832	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Konduskar/Phönix	Cloridrato de lidocaína m...	1202035-03	1
Krieger	Cloridrato de lidocaína m...	1612015-04	1
L10	Cloridrato de lidocaína m...	1612015-01	1
L10	Cloridrato de lidocaína m...	1612015-03	1
L12	Cloridrato de lidocaína m...	1505023-02	1
L12	Cloridrato de lidocaína m...	1606024-01	2
Lamotte/Noweda	Cloridrato de lidocaína m...	1622207	1
Mahendra Chem./ Phön...	Cloridrato de lidocaína m...	1411010-01	1
Mahendra Chem./Noweda	Cloridrato de lidocaína m...	1505023	1
Mahendra Chem.	Cloridrato de lidocaína m...	1411010-01	1
Merck	Cloridrato de lidocaína m...	K52817248	1
Moehns BCN, S.L.	Cloridrato de lidocaína m...	191350002	1
Moehs / Ebert	Cloridrato de lidocaína m...	15215201	1
Moehs / Gehe	Cloridrato de lidocaína m...	17292313	1
Moehs Catalana, S.L....	Cloridrato de lidocaína m...		1
Noweda 04.12.2019	Cloridrato de lidocaína m...	907012-01	1
Noweda 23.10.2019	Cloridrato de lidocaína m...	1808031-03	1
Noweda/apotec	Cloridrato de lidocaína m...	2201026-01	1
Noweda/Eurho 18,01,2...	Cloridrato de lidocaína m...	1907012-03	1
Noweda/EuRho	Cloridrato de lidocaína m...	2101034-03	1
Noweda/EuRo	Cloridrato de lidocaína m...	1612015-03	1
Noweda	Cloridrato de lidocaína m...	1108017-02	1
Noweda	Cloridrato de lidocaína m...	1202035-03	1
Noweda	Cloridrato de lidocaína m...	141101002	1
Noweda	Cloridrato de lidocaína m...	1606024-01	1
Noweda	Cloridrato de lidocaína m...	1606024-02	1
Noweda	Cloridrato de lidocaína m...	1612015-02	1
Noweda	Cloridrato de lidocaína m...	1612015-05	1
Noweda	Cloridrato de lidocaína m...	16222207	2
Noweda	Cloridrato de lidocaína m...	16222214	1
Noweda	Cloridrato de lidocaína m...	17204804	1
Noweda	Cloridrato de lidocaína m...	17292304	1
Noweda	Cloridrato de lidocaína m...	1808031-01	1
Noweda	Cloridrato de lidocaína m...	1808031-02	2
Noweda	Cloridrato de lidocaína m...	1808031-03	1
Noweda	Cloridrato de lidocaína m...	1812015-04	1
Noweda	Cloridrato de lidocaína m...	18179904	2
Noweda	Cloridrato de lidocaína m...	1907012_02	1
Noweda	Cloridrato de lidocaína m...	1907012-01	2
Noweda	Cloridrato de lidocaína m...	1907012-02	1
Noweda	Cloridrato de lidocaína m...	1907012-04	1
Noweda	Cloridrato de lidocaína m...	1913500010	1
Noweda	Cloridrato de lidocaína m...	191350007	2
Noweda	Cloridrato de lidocaína m...	20004451004	1
Noweda	Cloridrato de lidocaína m...	20004451008	1
Noweda	Cloridrato de lidocaína m...	2101034-01	2
Noweda	Cloridrato de lidocaína m...	2101034-02	1
Noweda	Cloridrato de lidocaína m...	22003202002	1
Noweda	Cloridrato de lidocaína m...	22003202007	2
Noweda	Cloridrato de lidocaína m...	2201026-01	1
Noweda	Cloridrato de lidocaína m...	2201026-02	1
Noweda	Cloridrato de lidocaína m...	2203202002	1
Noweda	Cloridrato de lidocaína m...	22102601	1
Noweda	Cloridrato de lidocaína m...	2211019-01	2
Noweda	Cloridrato de lidocaína m...	2211019-02	1
Noweda	Cloridrato de lidocaína m...	2273185	1
Noweda	Cloridrato de lidocaína m...	4914889	1
Noweda_31.07.2019	Cloridrato de lidocaína m...	1808031-02	1
Otto G. Apotec	Cloridrato de lidocaína m...	1907012-01	1
Otto Geilenkirchen Aachen	Cloridrato de lidocaína m...	20004307001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Parthe Apotheke	Cloridrato de lidocaína m...	192/20	1
Ph.Eur.10.0/Gehe	Cloridrato de lidocaína m...	1907012-02	1
Phoenix 03.12.2018	Cloridrato de lidocaína m...	1808031-01	1
PHOENIX 17.06.2014	Cloridrato de lidocaína m...	1403025-01	1
Phoenix 26.02.2014	Cloridrato de lidocaína m...	13118814	1
PHOENIX am 12.02.2014	Cloridrato de lidocaína m...	1202035-02	1
Phoenix	Cloridrato de lidocaína m...	1606024-02	1
Phoenix	Cloridrato de lidocaína m...	1612015-02	1
Phoenix	Cloridrato de lidocaína m...	16C09-B03-322144	1
Phoenix	Cloridrato de lidocaína m...	1808031-01	1
Phoenix	Cloridrato de lidocaína m...	1808031-02	3
Phoenix	Cloridrato de lidocaína m...	1808031-03	1
Phoenix	Cloridrato de lidocaína m...	1907012-01	3
Phoenix	Cloridrato de lidocaína m...	1907012-03	1
Phoenix	Cloridrato de lidocaína m...	1907012-04	1
Phoenix	Cloridrato de lidocaína m...	19e22-b01-191467	1
Phoenix	Cloridrato de lidocaína m...	200122101	1
Phoenix	Cloridrato de lidocaína m...	200562306	1
Phoenix	Cloridrato de lidocaína m...	2101034-01	1
Phoenix	Cloridrato de lidocaína m...	2101034-02	1
Phoenix	Cloridrato de lidocaína m...	2101034-03	1
Phoenix	Cloridrato de lidocaína m...	2201026-02	1
Phoenix	Cloridrato de lidocaína m...	2211019-01	2
Phoenix	Cloridrato de lidocaína m...	3238	1
Phönix Gotha	Cloridrato de lidocaína m...	1411010-02	1
Phönix/apo ident	Cloridrato de lidocaína m...	1808031-01	1
Phönix/EuRo	Cloridrato de lidocaína m...	1907012-03	1
Phönix	Cloridrato de lidocaína m...	1202035-03	1
Phönix	Cloridrato de lidocaína m...	12176103	1
phönix	Cloridrato de lidocaína m...	1505023-03	1
Phönix	Cloridrato de lidocaína m...	1606024-01	2
Phönix	Cloridrato de lidocaína m...	1612015-01	2
Phönix	Cloridrato de lidocaína m...	1612015-03	2
phönix	Cloridrato de lidocaína m...	16222207	2
Phönix	Cloridrato de lidocaína m...	1808031-02	1
Phönix	Cloridrato de lidocaína m...	18179904	1
Phönix	Cloridrato de lidocaína m...	1907012-01	3
Phönix	Cloridrato de lidocaína m...	1907012-02	4
PHÖNIX	Cloridrato de lidocaína m...	1907012-02	1
Phönix	Cloridrato de lidocaína m...	190701203	1
Phönix	Cloridrato de lidocaína m...	1907012-03	1
Phönix	Cloridrato de lidocaína m...	20004451002	1
Phönix	Cloridrato de lidocaína m...	21002505007	1
Phönix	Cloridrato de lidocaína m...	2101034-01	1
Phönix	Cloridrato de lidocaína m...	2101034-02	3
Phönix	Cloridrato de lidocaína m...	221019-01	1
Phönix	Cloridrato de lidocaína m...	2211019-02	1
Phönix	Cloridrato de lidocaína m...	B02-1969804	1
Phönix	Cloridrato de lidocaína m...	LDH/722031	1
Rondell Apotheke	Cloridrato de lidocaína m...	15215308	1
sana	Cloridrato de lidocaína m...	1403025-02	1
Sana	Cloridrato de lidocaína m...	2101034-03	1
Sanacorp	Cloridrato de lidocaína m...	1202035-01	3
Sanacorp	Cloridrato de lidocaína m...	13118807	1
Sanacorp	Cloridrato de lidocaína m...	1403025-01	1
Sanacorp	Cloridrato de lidocaína m...	1411010-01	1
Sanacorp	Cloridrato de lidocaína m...	14J07-B04-299434	2
Sanacorp	Cloridrato de lidocaína m...	150502302	1
Sanacorp	Cloridrato de lidocaína m...	15215309	1
Sanacorp	Cloridrato de lidocaína m...	15215312	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Cloridrato de lidocaína m…	15299513	1
Sanacorp	Cloridrato de lidocaína m…	1606024-02	1
Sanacorp	Cloridrato de lidocaína m…	17204804	1
Sanacorp	Cloridrato de lidocaína m…	17292307	1
Sanacorp	Cloridrato de lidocaína m…	17292313	1
Sanacorp	Cloridrato de lidocaína m…	1808031-02	1
Sanacorp	Cloridrato de lidocaína m…	18179911	1
Sanacorp	Cloridrato de lidocaína m…	18179914	1
Sanacorp	Cloridrato de lidocaína m…	19135103	5
Sanacorp	Cloridrato de lidocaína m…	2101034-01	1
Sanacorp	Cloridrato de lidocaína m…	21I17-B03-213766	1
Sanacorp	Cloridrato de lidocaína m…	22003202008	1
Sanacorp	Cloridrato de lidocaína m…	2201023-02	1
Sanacorp	Cloridrato de lidocaína m…	2201026-01	2
Sanacorp	Cloridrato de lidocaína m…	2211019-01	1
Sanacorp	Cloridrato de lidocaína m…	2211019-03	2
Sanacorp	Cloridrato de lidocaína m…	22H22-B03-224257	1
Sanacorp	Cloridrato de lidocaína m…	23003452002	1
Sanacorp	Cloridrato de lidocaína m…	23003452004	1
siehe Protokoll	Cloridrato de lidocaína m…	1606024-01	1
Swati / Noweda	Cloridrato de lidocaína m…	1606024-01	1
Swati /Nowreda	Cloridrato de lidocaína m…	1907012-03	1
Swati Spentose Priva…	Cloridrato de lidocaína m…	1808031-01	1
swati spentose priva…	Cloridrato de lidocaína m…	210103401	1
Swati Spentose Priva…	Cloridrato de lidocaína m…	1907012-04	1
Swati Spentose Private	Cloridrato de lidocaína m…	2101034-01	1
Swati Spentose Private	Cloridrato de lidocaína m…	2101034-02	1
Swati/Noweda	Cloridrato de lidocaína m…	LDH/116007	1
SWATI/Noweda	Cloridrato de lidocaína m…	LDH719007	1
SWATI/Phoenix	Cloridrato de lidocaína m…	LDH/719007	6
SWATI/Phoenix	Cloridrato de lidocaína m…	LDH/720023	3
Swati/Phönix	Cloridrato de lidocaína m…	21A12-B04-203052	1
SWATI/Phönix	Cloridrato de lidocaína m…	LDH/719007	1
Swati/Sanacorp	Cloridrato de lidocaína m…	2201026-01	1
Swati	Cloridrato de lidocaína m…	1606024-01	1
Symbiotica	Cloridrato de lidocaína m…	1606024-02	1

- 232 408 spectra from 1515 *Apo-Ident* customers from a total of 48 770 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de lidocaína monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de lidocaína monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	620	0	201 464
Type C	0	3650	9	232 408

The substance/substance group *Cloridrato de lidocaína monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.7540 % (> 99.6720 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20882	20882	0,00	192,57
21613	23807	8,97	188,22
21770	21770	0,00	198,52
23807	23807	0,00	193,87
24776	24776	0,00	202,28
25446	21770	11,40	204,54
26028	26028	0,00	211,62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de lisina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20385-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de lisina; Lisina, cloridrato; Lysini hydrochloridum

Special notes

When selecting the *Cloridrato de lisina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de lisina	8	11	8

Second-stage model

For differentiation of the substance/substance group *Cloridrato de lisina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de lisina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Levocarnitina	95,78	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de lisina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de lisina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de lisina	1611021	22865	40	20161202*
Euro OTC	Cloridrato de lisina	1708009	23698	40	20170922*
Euro OTC	Cloridrato de lisina	1805030	24123	40	20180611*
Euro OTC	Cloridrato de lisina	2003009	25128	40	20200403*
Euro OTC	Cloridrato de lisina	2010008	25459	40	20201124*
Euro OTC	Cloridrato de lisina	2105002	25675	40	20210527*
Fagron	Cloridrato de lisina	15B09-B06-304170	21963	60	20150220
Fagron	Cloridrato de lisina	14H20-B03-301894	21983	60	AR-16-FG-005856-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 360 spectra of 8 reference samples from the substance/substance group *Cloridrato de lisina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 500 spectra of 14 reference samples from the substance/substance group *Cloridrato de lisina*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de lisina	1603011	22527	40
Euro OTC	Cloridrato de lisina	1902008	24622	40
Euro OTC	Cloridrato de lisina	1907038	24809	40
Euro OTC	Cloridrato de lisina	2006008	25352	40
Euro OTC	Cloridrato de lisina	2205013	26197	40
Euro OTC	Cloridrato de lisina	2302003	26657	40
Euro OTC	Cloridrato de lisina	2406017	27368	40
Fagron	Cloridrato de lisina	12B14-N08	20735	40
Fagron	Cloridrato de lisina	22J11-B06	26448	40
Fagron	Cloridrato de lisina	23E18-B02-231717	26821	40
Fagron	Cloridrato de lisina	24E06-B24-238724	27413	40
Euro OTC	Cloridrato de lisina	2205013	26197SI	20
Euro OTC	Cloridrato de lisina	2302003	26657SI	20
Fagron	Cloridrato de lisina	23E18-B02-231717	26821SI	20

- 201 584 spectra from a total of 4034 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 22 spectra from 4 *Apo-Ident* customers from 9 batches from the substance/substance group *Cloridrato de lisina*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de lisina	1708009-01	2
Euro OTC	Cloridrato de lisina	1805030-01	1
Euro OTC	Cloridrato de lisina	1907038-01	1
Euro OTC	Cloridrato de lisina	2006008-01	11
Euro OTC	Cloridrato de lisina	2105002-02	2
Euro OTC	Cloridrato de lisina	2205013-01	2
Euro OTC	Cloridrato de lisina	gjjhgjhkj	1
Fagron	Cloridrato de lisina	14H20-B03-301894	1
Fagron	Cloridrato de lisina	21H23-B03-213624	1

- 236 045 spectra from 1515 *Apo-Ident* customers from a total of 49 251 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de lisina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de lisina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	460	40	201 584
Type C	0	22	0	236 045

The substance/substance group *Cloridrato de lisina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	92.0000 % (> 91.4000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 72.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21963	21983	6,75	203,00
21983	21983	0,00	203,13
22865	22865	0,00	198,14
23698	23698	0,00	201,92
24123	24123	0,00	198,55
25128	25128	0,00	203,75
25459	25459	0,00	195,01
25675	25675	0,00	146,61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de mepivacaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20710-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de mepivacaína; Mepivacaína, cloridrato; Mepivacaini hydrochloridum

Special notes

When selecting the *Cloridrato de mepivacaína* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de mepivacaína	5	1	10

Second-stage model

For differentiation of the substance/substance group *Cloridrato de mepivacaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de mepivacaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tretinoína	51,31	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de mepivacaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de mepivacaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de mepivacaína	12A20-N12	20710	40	1401555
Fagron	Cloridrato de mepivacaína	13L04-B07-297077	21672	60	AR-15-FG-007876-01
Fagron	Cloridrato de mepivacaína	19F25-B02-365217	24950	40	2007301
Fagron	Cloridrato de mepivacaína	20D24-F01-370950	25368	40	20200610
Fagron	Cloridrato de mepivacaína	22C04-B01-217581	26733	40	20220603
Fagron	Cloridrato de mepivacaína	22C04-B01-217581	26733SI	20	20220603

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Cloridrato de mepivacaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 722 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Cloridrato de mepivacaína*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de mepivacaína	15I16-B01-322906	23212	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 13 spectra from 8 *Apo-Ident* customers from 11 batches from the substance/substance group *Cloridrato de mepivacaína*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de mepivacaína	13G05-N02	1
Fagron	Cloridrato de mepivacaína	12E31-B40-305570	1
Fagron	Cloridrato de mepivacaína	12F20-N07	1
Fagron	Cloridrato de mepivacaína	13G05N02	1
Fagron	Cloridrato de mepivacaína	13G05-N02	1
Fagron	Cloridrato de mepivacaína	15E04-B04-330855	1
Fagron	Cloridrato de mepivacaína	15I16-B01	1
Fagron	Cloridrato de mepivacaína	15I16-B01-341738	1
Fagron	Cloridrato de mepivacaína	15I16-B01-356826	1
Fagron	Cloridrato de mepivacaína	15I16-B-325107	2
Fagron	Cloridrato de mepivacaína	19F25-B02	1
Sanacorp	Cloridrato de mepivacaína	19F25-B02-365217	1

- 236 054 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de mepivacaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de mepivacaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	40	0	202 044
Type C	0	13	0	236 054

The substance/substance group *Cloridrato de mepivacaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20710	20710	0,00	53,15
21672	21672	0,00	52,81
24950	24950	0,00	53,99
25368	21672	10,83	53,76
26733	24950	25,80	51,31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de metadona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20306-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de metadona; Metadona, cloridrato; Methadoni hydrochloridum

Special notes

When selecting the *Cloridrato de metadona* substance/substance group, the following information is displayed to the user:

- Nota sobre identificação do cloridrato de metadona: O cloridrato de levometadona é uma substância semelhante que não está incluída na base de dados. Pode ser necessário fazer uma análise de identidade adicional, medir o ponto de fusão!

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de metadona	7	4	383

Second-stage model

For differentiation of the substance/substance group *Cloridrato de metadona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de metadona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de difenidramina	54,75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de metadona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de metadona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de metadona	12344818	21170	40	0914E-02949
Caelo	Cloridrato de metadona	12344818	21170SI	60	0914E-02949
Caelo	Cloridrato de metadona	15244715	22417	60	1516A-02949
Caelo	Cloridrato de metadona	15244715	22417SI	60	1516A-02949
Fagron	Cloridrato de metadona	13J24-B06	21172	40	0914F-02949
Fagron	Cloridrato de metadona	13J24-B06	21172SI	60	0914F-02949
Fagron	Cloridrato de metadona	15E29-B02-313098	22428	60	1516B-02949
Fagron	Cloridrato de metadona	15E29-B02-313098	22428SI	60	1516B-02949
Fagron	Cloridrato de metadona	16F24-B02-323183	23485	40	1917Q-02949
Th. Geyer	Cloridrato de metadona	67033	21174	40	0914G-02949
Th. Geyer	Cloridrato de metadona	67033	21174SI	60	0914G-02949
Th. Geyer	Cloridrato de metadona	67047	21176	40	0914H-02949
Th. Geyer	Cloridrato de metadona	67047	21176SI	60	0914H-02949

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 680 spectra of 13 reference samples from the substance/substance group *Cloridrato de metadona*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 282 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 360 spectra of 9 reference samples from the substance/substance group *Cloridrato de metadona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de metadona	16135309	23484	40
Caelo	Cloridrato de metadona	18132413	24655	40
Fagron	Cloridrato de metadona	18G02-B02-355990	24654	40
Th. Geyer	Cloridrato de metadona	067055	23483	40
Caelo	Cloridrato de metadona	16135309	23484SI	40
Caelo	Cloridrato de metadona	18132413	24655SI	40
Fagron	Cloridrato de metadona	16F24-B02-323183	23485SI†	40
Fagron	Cloridrato de metadona	18G02-B02-355990	24654SI	40
Th. Geyer	Cloridrato de metadona	067055	23483SI	40

- 201 724 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1154 spectra from 418 *Apo-Ident* customers from 399 batches from the substance/substance group *Cloridrato de metadona*.

- Among them are spectra of independent samples from 383 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de metadona	18132403	1
	Cloridrato de metadona	21003277011	1
	Cloridrato de metadona	21003277014	1
	Cloridrato de metadona	21003277020	1
	Cloridrato de metadona	21003277024	7
	Cloridrato de metadona	21H25-F02-380291	1
	Cloridrato de metadona	22E02-F04	1
	Cloridrato de metadona	22E02-F04-382503	1
	Cloridrato de metadona	22E02-F04-382620	2
	Cloridrato de metadona	23001353006	1
	Cloridrato de metadona	23001356001	1
	Cloridrato de metadona	23003258005	1
	Cloridrato de metadona	23A25-F02-384693	1
	Cloridrato de metadona	23A25-F02-384698	2
	Cloridrato de metadona	23A25-F02-384702	2
	Cloridrato de metadona	70617	1
AHD	Cloridrato de metadona	12344812	1
Anzag	Cloridrato de metadona	21003277024	1
BLS Analytik GmbH	Cloridrato de metadona	70245	7
BLS	Cloridrato de metadona	70245	1
BLS-Analytik/Sanacorp	Cloridrato de metadona	67055	3
Bombastus	Cloridrato de metadona	14C24-B01-292858	6
Bombastus	Cloridrato de metadona	16135326	1
Caelo	Cloridrato de metadona		2
Caelo	Cloridrato de metadona	10076407	1
Caelo	Cloridrato de metadona	1081801	1
Caelo	Cloridrato de metadona	11021904	1
Caelo	Cloridrato de metadona	11227507	1
Caelo	Cloridrato de metadona	12171902	1
Caelo	Cloridrato de metadona	12171906	2
Caelo	Cloridrato de metadona	12171907	1
Caelo	Cloridrato de metadona	12171914	1
Caelo	Cloridrato de metadona	12171918	1
Caelo	Cloridrato de metadona	12344802	1
Caelo	Cloridrato de metadona	12344807	1
Caelo	Cloridrato de metadona	12344812	1
Caelo	Cloridrato de metadona	12344814	2
Caelo	Cloridrato de metadona	12344816	3
Caelo	Cloridrato de metadona	12344818	1
Caelo	Cloridrato de metadona	12344819	1
Caelo	Cloridrato de metadona	12H07-N05	1
Caelo	Cloridrato de metadona	13266501	1
Caelo	Cloridrato de metadona	13266502	2
Caelo	Cloridrato de metadona	13266504	2
Caelo	Cloridrato de metadona	13266505	4
Caelo	Cloridrato de metadona	13266511	2
Caelo	Cloridrato de metadona	13266514	1
Caelo	Cloridrato de metadona	13266515	1
Caelo	Cloridrato de metadona	13266518	3
Caelo	Cloridrato de metadona	13266521	1
Caelo	Cloridrato de metadona	1327H051	1
Caelo	Cloridrato de metadona	13F17-N02	2
Caelo	Cloridrato de metadona	14C24-B01-292860	1
Caelo	Cloridrato de metadona	15215501	1
Caelo	Cloridrato de metadona	15244701	1
Caelo	Cloridrato de metadona	15244702	1
Caelo	Cloridrato de metadona	15244704	3
Caelo	Cloridrato de metadona	15244705	2
Caelo	Cloridrato de metadona	15244706	3
Caelo	Cloridrato de metadona	15244709	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de metadona	15244710	4
Caelo	Cloridrato de metadona	15244713	4
Caelo	Cloridrato de metadona	15244715	2
Caelo	Cloridrato de metadona	15244717	6
Caelo	Cloridrato de metadona	15244718	1
Caelo	Cloridrato de metadona	15244720	1
Caelo	Cloridrato de metadona	15I24-B07-317266	1
Caelo	Cloridrato de metadona	1608H002	1
Caelo	Cloridrato de metadona	1613529	1
Caelo	Cloridrato de metadona	16135301	1
Caelo	Cloridrato de metadona	16135302	1
Caelo	Cloridrato de metadona	16135303	1
Caelo	Cloridrato de metadona	16135305	6
Caelo	Cloridrato de metadona	16135307	2
Caelo	Cloridrato de metadona	16135308	4
Caelo	Cloridrato de metadona	16135309	1
Caelo	Cloridrato de metadona	16135310	4
Caelo	Cloridrato de metadona	16135311	4
Caelo	Cloridrato de metadona	16135312	3
Caelo	Cloridrato de metadona	16135315	1
Caelo	Cloridrato de metadona	16135316	2
Caelo	Cloridrato de metadona	16135317	2
Caelo	Cloridrato de metadona	16135318	7
Caelo	Cloridrato de metadona	16135319	2
Caelo	Cloridrato de metadona	16135322	1
Caelo	Cloridrato de metadona	16135323	1
Caelo	Cloridrato de metadona	16135324	6
Caelo	Cloridrato de metadona	16135325	4
Caelo	Cloridrato de metadona	16135326	7
Caelo	Cloridrato de metadona	16135327	12
Caelo	Cloridrato de metadona	16135328	1
Caelo	Cloridrato de metadona	16135329	12
Caelo	Cloridrato de metadona	16135330	4
Caelo	Cloridrato de metadona	16135332	11
Caelo	Cloridrato de metadona	16208016	1
Caelo	Cloridrato de metadona	16F24-B02-323184	1
Caelo	Cloridrato de metadona	17011406	1
Caelo	Cloridrato de metadona	17051801	1
Caelo	Cloridrato de metadona	1718H028	4
Caelo	Cloridrato de metadona	171920-0004	1
Caelo	Cloridrato de metadona	1723	1
Caelo	Cloridrato de metadona	172329504	1
Caelo	Cloridrato de metadona	1723509	1
Caelo	Cloridrato de metadona	17239501	1
Caelo	Cloridrato de metadona	17239502	2
Caelo	Cloridrato de metadona	17239503	4
Caelo	Cloridrato de metadona	17239504	8
Caelo	Cloridrato de metadona	17239506	9
Caelo	Cloridrato de metadona	17239507	4
Caelo	Cloridrato de metadona	17239508	3
Caelo	Cloridrato de metadona	17239510	6
Caelo	Cloridrato de metadona	17239512	11
Caelo	Cloridrato de metadona	17239514	1
Caelo	Cloridrato de metadona	17239518	6
Caelo	Cloridrato de metadona	1729504	1
Caelo	Cloridrato de metadona	177239518	1
Caelo	Cloridrato de metadona	17C24-B05	1
Caelo	Cloridrato de metadona	17I15-B02-339523	2
Caelo	Cloridrato de metadona	17I15-B02-343150	1
Caelo	Cloridrato de metadona	180219MC/17239506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de metadona	18132403	5
Caelo	Cloridrato de metadona	18132404	2
Caelo	Cloridrato de metadona	18132405	5
Caelo	Cloridrato de metadona	18132405P-190225-10	1
Caelo	Cloridrato de metadona	18132405P-190527-1	1
Caelo	Cloridrato de metadona	18132406	3
Caelo	Cloridrato de metadona	18132407	2
Caelo	Cloridrato de metadona	18132408	12
Caelo	Cloridrato de metadona	18132409	1
Caelo	Cloridrato de metadona	18132412	6
Caelo	Cloridrato de metadona	18132413	8
Caelo	Cloridrato de metadona	18132413P-190709-2	1
Caelo	Cloridrato de metadona	18132413P-190916-1	1
Caelo	Cloridrato de metadona	18132416	1
Caelo	Cloridrato de metadona	18132417	7
Caelo	Cloridrato de metadona	1816601	1
Caelo	Cloridrato de metadona	18186601	12
Caelo	Cloridrato de metadona	18186601P-181001-4	1
Caelo	Cloridrato de metadona	18186604	3
Caelo	Cloridrato de metadona	18186607	4
Caelo	Cloridrato de metadona	18186608	10
Caelo	Cloridrato de metadona	18C01-B05-350571	2
Caelo	Cloridrato de metadona	18c01b05350572	1
Caelo	Cloridrato de metadona	18g02-b02355992	1
Caelo	Cloridrato de metadona	18g02-b02-355992	1
Caelo	Cloridrato de metadona	190000787013	1
Caelo	Cloridrato de metadona	19000787001	7
Caelo	Cloridrato de metadona	19000787001P2006221	1
Caelo	Cloridrato de metadona	19000787002	1
Caelo	Cloridrato de metadona	19000787003	5
Caelo	Cloridrato de metadona	19000787004	4
Caelo	Cloridrato de metadona	19000787008	4
Caelo	Cloridrato de metadona	19000787013	1
Caelo	Cloridrato de metadona	19000787016	2
Caelo	Cloridrato de metadona	19000824003	1
Caelo	Cloridrato de metadona	19000824004	1
Caelo	Cloridrato de metadona	19011913	1
Caelo	Cloridrato de metadona	190603141F	1
Caelo	Cloridrato de metadona	191494001	7
Caelo	Cloridrato de metadona	191494003	7
Caelo	Cloridrato de metadona	19149401	2
Caelo	Cloridrato de metadona	19149402	7
Caelo	Cloridrato de metadona	19149402P-191223-1	1
Caelo	Cloridrato de metadona	19149403	1
Caelo	Cloridrato de metadona	19149404	1
Caelo	Cloridrato de metadona	19149406	3
Caelo	Cloridrato de metadona	19149406P-200323-2	1
Caelo	Cloridrato de metadona	19149407	2
Caelo	Cloridrato de metadona	19149409	3
Caelo	Cloridrato de metadona	19D09-B03-3645508	1
Caelo	Cloridrato de metadona	20170728/Ma2	1
Caelo	Cloridrato de metadona	21000271001	1
Caelo	Cloridrato de metadona	21000271002	1
Caelo	Cloridrato de metadona	21000271004	1
Caelo	Cloridrato de metadona	21000271007	2
Caelo	Cloridrato de metadona	21000271011	3
Caelo	Cloridrato de metadona	21000271013	2
Caelo	Cloridrato de metadona	21000271019	7
Caelo	Cloridrato de metadona	21003277001	1
Caelo	Cloridrato de metadona	21003277005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de metadona	21003277006	8
Caelo	Cloridrato de metadona	21003277009	6
Caelo	Cloridrato de metadona	21003277011	1
Caelo	Cloridrato de metadona	21003277014	2
Caelo	Cloridrato de metadona	21003277020	1
Caelo	Cloridrato de metadona	220901smi//21000271019	1
Caelo	Cloridrato de metadona	23021802	1
Caelo	Cloridrato de metadona	25111701	1
Caelo	Cloridrato de metadona	28041725	1
Caelo	Cloridrato de metadona	28061702	1
Caelo	Cloridrato de metadona	2912161	1
Caelo	Cloridrato de metadona	31011901	1
Caelo	Cloridrato de metadona	3111806	1
Caelo	Cloridrato de metadona	57(18132413)	1
Caelo	Cloridrato de metadona	58(18132417)	1
Caelo	Cloridrato de metadona	61(19000787001)	1
Caelo	Cloridrato de metadona	70245	1
Caelo	Cloridrato de metadona	7091708	1
Caelo	Cloridrato de metadona	70925	1
Caelo	Cloridrato de metadona	LOT067055	1
Caelo	Cloridrato de metadona	M260813	1
Caeol/Phönix	Cloridrato de metadona	17239506	1
Caesar & Loretz GmbH...	Cloridrato de metadona	18132403	1
Caesar & Loretz GmbH...	Cloridrato de metadona	18132417	1
Caesar & Loretz GmbH...	Cloridrato de metadona	18186608	1
Caesar & Loretz GmbH/	Cloridrato de metadona	191494	2
Caesar & Loretz GmbH/Gehe	Cloridrato de metadona	19000787012	2
Caesar & Loretz GmbH/Gerx	Cloridrato de metadona	21000271013	1
Caesar & Loretz GmbH...	Cloridrato de metadona	19149402	1
Caesar & Loretz GmbH...	Cloridrato de metadona	18186603	2
Caesar & Loretz GmbH...	Cloridrato de metadona	19000787004	1
Caesar & Loretz GmbH...	Cloridrato de metadona	19000787008	1
Caesar & Loretz GmbH...	Cloridrato de metadona	19149405	1
Caesar & Loretz GmbH...	Cloridrato de metadona	18132408	1
Caesar & Loretz GmbH	Cloridrato de metadona	18132403	1
Caesar & Loretz GmbH	Cloridrato de metadona	18132404	1
Caesar & Loretz GmbH	Cloridrato de metadona	18132406	1
Caesar & Loretz GmbH	Cloridrato de metadona	18132407	1
Caesar & Loretz GmbH	Cloridrato de metadona	18132408	3
Caesar & Loretz GmbH	Cloridrato de metadona	18132412	2
Caesar & Loretz GmbH	Cloridrato de metadona	18132413	3
Caesar & Loretz GmbH	Cloridrato de metadona	18132416	3
Caesar & Loretz GmbH	Cloridrato de metadona	18132417	3
Caesar & Loretz GmbH	Cloridrato de metadona	18186604	1
Caesar & Loretz GmbH	Cloridrato de metadona	18186605	1
Caesar & Loretz GmbH	Cloridrato de metadona	18186607	1
Caesar & Loretz GmbH	Cloridrato de metadona	19000787003	1
Caesar & Loretz GmbH	Cloridrato de metadona	19000787005	3
Caesar & Loretz GmbH	Cloridrato de metadona	19000787008	3
Caesar & Loretz GmbH	Cloridrato de metadona	19000787013	1
Caesar & Loretz GmbH	Cloridrato de metadona	19000824004	2
Caesar & Loretz GmbH	Cloridrato de metadona	191494001	1
Caesar & Loretz GmbH	Cloridrato de metadona	191494003	3
CAESAR & LORETZ GMBH	Cloridrato de metadona	191494003	1
Caesar & Loretz GmbH	Cloridrato de metadona	20D09-F05-371481	1
Caesar & Loretz GmbH	Cloridrato de metadona	21000271002	3
Caesar & Loretz GmbH	Cloridrato de metadona	21000271004	1
Caesar & Loretz GmbH	Cloridrato de metadona	21000271007	1
Caesar & Loretz GmbH	Cloridrato de metadona	21000271009	4
Caesar & Loretz GmbH	Cloridrato de metadona	21000271010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de metadona	21000271011	2
Caesar & Loretz GmbH	Cloridrato de metadona	21000271012	1
Caesar & Loretz GmbH	Cloridrato de metadona	21000271017	3
Caesar & Loretz GmbH	Cloridrato de metadona	21003277006	5
Caesar & Loretz GmbH	Cloridrato de metadona	21003277009	1
Caesar & Loretz GmbH	Cloridrato de metadona	21003277010	1
Caesar & Loretz GmbH	Cloridrato de metadona	21003277015	1
Caesar & Loretz GmbH	Cloridrato de metadona	F01-3764906	2
Caesar & Loretz GmbH	Cloridrato de metadona	f05-3714801	1
Caesar & Loretz	Cloridrato de metadona	17239506	1
Caesar und Loretz GmbH	Cloridrato de metadona	18132412	1
Caesar und Loretz GmbH	Cloridrato de metadona	19149402	1
Cealo/ Anzag	Cloridrato de metadona	16135326	3
Cealo	Cloridrato de metadona	21000271007	1
Cordes/Alia	Cloridrato de metadona	19000787008	1
Dr. Wolff	Cloridrato de metadona	16F24-B02	1
Ebert & Jacobi	Cloridrato de metadona	16135308	1
Ebert-Jacobi	Cloridrato de metadona	16135306	1
Euro OTC	Cloridrato de metadona	14C24-B01	1
Euro OTC	Cloridrato de metadona	16135304	5
Euro OTC	Cloridrato de metadona	16135318	1
Faagron	Cloridrato de metadona	1437H011	1
Fagro/ Noweda	Cloridrato de metadona	17/15-B02-339527	1
Fagro//Noweda	Cloridrato de metadona	15/24-B07-317267	1
Fagro/Jenne	Cloridrato de metadona	17I15-B02-339525	2
Fagron	Cloridrato de metadona		2
Fagron	Cloridrato de metadona	11D07-N09	1
Fagron	Cloridrato de metadona	11G11-N02	1
Fagron	Cloridrato de metadona	1207h057	1
Fagron	Cloridrato de metadona	1213E-02949	1
Fagron	Cloridrato de metadona	1225H008	1
Fagron	Cloridrato de metadona	12A05-No2	1
Fagron	Cloridrato de metadona	12b21-n03	1
Fagron	Cloridrato de metadona	12B21N03	1
Fagron	Cloridrato de metadona	12H07-N05	3
Fagron	Cloridrato de metadona	12H07-N07	1
Fagron	Cloridrato de metadona	1316H037	4
Fagron	Cloridrato de metadona	1327h051	1
Fagron	Cloridrato de metadona	13B06-N02	5
Fagron	Cloridrato de metadona	13F17-N02	4
Fagron	Cloridrato de metadona	13I24-B06-286908	1
Fagron	Cloridrato de metadona	13J24-B06-286906	1
Fagron	Cloridrato de metadona	13J24-B06-286907	1
Fagron	Cloridrato de metadona	13J24-B06-286908	1
Fagron	Cloridrato de metadona	13J24B06286910	1
Fagron	Cloridrato de metadona	1409H043	1
Fagron	Cloridrato de metadona	1437H012	2
Fagron	Cloridrato de metadona	14C24-B01	1
Fagron	Cloridrato de metadona	14C24-B01-292857	4
Fagron	Cloridrato de metadona	14H15-B01	1
Fagron	Cloridrato de metadona	14H15-B01-299381	1
Fagron	Cloridrato de metadona	14H15-B01-299382	6
Fagron	Cloridrato de metadona	15/24-B07-313517	1
Fagron	Cloridrato de metadona	1514H042	3
Fagron	Cloridrato de metadona	15244704	1
Fagron	Cloridrato de metadona	15-B02-339525	1
Fagron	Cloridrato de metadona	15-B02-343150	1
Fagron	Cloridrato de metadona	15B24-B02-304724	6
Fagron	Cloridrato de metadona	15B24-B02-313097	1
Fagron	Cloridrato de metadona	15E29_B02_309070	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de metadona	15E29-B02-309070	2
Fagron	Cloridrato de metadona	15E29-B02-313031	1
Fagron	Cloridrato de metadona	15E29-B02-313098	3
Fagron	Cloridrato de metadona	15I24-B07	1
Fagron	Cloridrato de metadona	1608H002	1
Fagron	Cloridrato de metadona	16B16-B02-318420	3
Fagron	Cloridrato de metadona	16F24-B02-323182	1
Fagron	Cloridrato de metadona	16f24-b02-323184	1
Fagron	Cloridrato de metadona	16F24B02323184	2
Fagron	Cloridrato de metadona	16F24-B02-323185	1
Fagron	Cloridrato de metadona	16F24-B02-323186	1
Fagron	Cloridrato de metadona	16F24-B02-326207	3
Fagron	Cloridrato de metadona	16F24-B02-329935	1
Fagron	Cloridrato de metadona	16K01B04	1
Fagron	Cloridrato de metadona	16K01-B04	2
Fagron	Cloridrato de metadona	16k01-b04-329933	1
Fagron	Cloridrato de metadona	16K01-B04-329933	3
Fagron	Cloridrato de metadona	16K01-B04-329934	2
Fagron	Cloridrato de metadona	16K01-B04-329936	1
Fagron	Cloridrato de metadona	16-k01-B04-329937	1
Fagron	Cloridrato de metadona	16K01-B04-329937	1
Fagron	Cloridrato de metadona	17/15-B02	1
Fagron	Cloridrato de metadona	17/15-B02-339521	4
Fagron	Cloridrato de metadona	17/15-B02-343150	1
Fagron	Cloridrato de metadona	17/15-B02-343153	1
Fagron	Cloridrato de metadona	170427MH/1608H002	1
Fagron	Cloridrato de metadona	17105-B02	1
Fagron	Cloridrato de metadona	1715-B02-339523	1
Fagron	Cloridrato de metadona	1715-B02-339525	2
Fagron	Cloridrato de metadona	1715-B02-343150	1
Fagron	Cloridrato de metadona	1715-B02-343151	1
Fagron	Cloridrato de metadona	1718H028	10
Fagron	Cloridrato de metadona	1718HO28	1
Fagron	Cloridrato de metadona	171920-0009	1
Fagron	Cloridrato de metadona	17c24-b05	1
Fagron	Cloridrato de metadona	17C24-B05	1
Fagron	Cloridrato de metadona	17c24b05334309	1
Fagron	Cloridrato de metadona	17C24-B05-334309	6
Fagron	Cloridrato de metadona	17C24-B05-334311	2
Fagron	Cloridrato de metadona	17C24-B05-335711	11
Fagron	Cloridrato de metadona	17C24-B05-335712	1
Fagron	Cloridrato de metadona	17C24-B-335711	1
Fagron	Cloridrato de metadona	17c24-bo5334311	1
Fagron	Cloridrato de metadona	17I15-B02	8
Fagron	Cloridrato de metadona	17I15-B02-339521	6
Fagron	Cloridrato de metadona	17I15-B02-339523	6
Fagron	Cloridrato de metadona	17I15-B02-339528	1
Fagron	Cloridrato de metadona	17I15-B02-339529	2
Fagron	Cloridrato de metadona	17I15-B02-343150	4
Fagron	Cloridrato de metadona	17I15-B02-343151	2
Fagron	Cloridrato de metadona	17I15-B02-343153	1
Fagron	Cloridrato de metadona	17I15W02	1
Fagron	Cloridrato de metadona	17l15-B02	1
Fagron	Cloridrato de metadona	17l15-B02-339521	1
Fagron	Cloridrato de metadona	17l15-B02-343153	1
Fagron	Cloridrato de metadona	17l15-B02-343154	2
Fagron	Cloridrato de metadona	1801h011	1
Fagron	Cloridrato de metadona	1801H011	3
Fagron	Cloridrato de metadona	1801h11	1
Fagron	Cloridrato de metadona	1814H016	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de metadona	1847H015	6
Fagron	Cloridrato de metadona	18C01-B05-346737	6
Fagron	Cloridrato de metadona	18C01-B05-350571	7
Fagron	Cloridrato de metadona	18c01-b05-350572	1
Fagron	Cloridrato de metadona	18C01-B05-350572	1
Fagron	Cloridrato de metadona	18C01-B05-350573	2
Fagron	Cloridrato de metadona	18G02-B02	7
Fagron	Cloridrato de metadona	18G02B02351285	2
Fagron	Cloridrato de metadona	18G02-B02-351285	1
Fagron	Cloridrato de metadona	18G02-B02-35590	1
Fagron	Cloridrato de metadona	18G02-B02-355989	7
Fagron	Cloridrato de metadona	18G02-B02-355990	7
Fagron	Cloridrato de metadona	18G02-B02-355991	1
Fagron	Cloridrato de metadona	18G02-B02-355993	2
Fagron	Cloridrato de metadona	18G02-B02-355994	1
Fagron	Cloridrato de metadona	19149401	1
Fagron	Cloridrato de metadona	1914H016	3
Fagron	Cloridrato de metadona	19D09-B03	7
Fagron	Cloridrato de metadona	19D09-B03_364513	1
Fagron	Cloridrato de metadona	19D09-B03_364514	1
Fagron	Cloridrato de metadona	19D09-B03-364513	8
Fagron	Cloridrato de metadona	19D09-B03-364514	3
Fagron	Cloridrato de metadona	19D09-B03-364516	2
Fagron	Cloridrato de metadona	19D09-B03-364517	4
Fagron	Cloridrato de metadona	19D09-B03-364518	1
Fagron	Cloridrato de metadona	19D09-B03-364519	1
Fagron	Cloridrato de metadona	19D09-B03-364558	4
Fagron	Cloridrato de metadona	19D09-B03-364559	1
Fagron	Cloridrato de metadona	19D09-B03-364560	1
Fagron	Cloridrato de metadona	19D9-B03-364514	1
Fagron	Cloridrato de metadona	200000000	1
Fagron	Cloridrato de metadona	20130912-6	1
Fagron	Cloridrato de metadona	20A09F05	1
Fagron	Cloridrato de metadona	20A09-F05	5
Fagron	Cloridrato de metadona	20A09-F05-370755	5
Fagron	Cloridrato de metadona	20A09-F05-370757	2
Fagron	Cloridrato de metadona	20A09-F05-370758	1
Fagron	Cloridrato de metadona	20A09-F05-370759	1
Fagron	Cloridrato de metadona	20A09-F05-371479	1
Fagron	Cloridrato de metadona	20D09F05	2
Fagron	Cloridrato de metadona	20D09-F05	3
Fagron	Cloridrato de metadona	20D09-F05-370589	4
Fagron	Cloridrato de metadona	20D09-F05-370590	1
Fagron	Cloridrato de metadona	20D09-F05-371480	1
Fagron	Cloridrato de metadona	21002144002	1
Fagron	Cloridrato de metadona	2117H030	3
Fagron	Cloridrato de metadona	211BH003	1
Fagron	Cloridrato de metadona	21A06-F01	3
Fagron	Cloridrato de metadona	21A06-F01-376496	1
Fagron	Cloridrato de metadona	21A06-F01-376497	2
Fagron	Cloridrato de metadona	21A06-F02	1
Fagron	Cloridrato de metadona	21A06-F02-376492	3
Fagron	Cloridrato de metadona	21G14-F06	2
Fagron	Cloridrato de metadona	21G14-F06-379151	1
Fagron	Cloridrato de metadona	21G14-F06-379152	2
Fagron	Cloridrato de metadona	21G14-F06-379154	1
Fagron	Cloridrato de metadona	21H25-F02	2
Fagron	Cloridrato de metadona	21H25-F02-380291	1
Fagron	Cloridrato de metadona	21H25-F02-380953	1
Fagron	Cloridrato de metadona	21H25-F02-380954	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de metadona	21H25-F02-380956	1
Fagron	Cloridrato de metadona	22E02-F04-382503	2
Fagron	Cloridrato de metadona	25091307	1
Fagron	Cloridrato de metadona	25091406	1
Fagron	Cloridrato de metadona	2877	1
Fagron	Cloridrato de metadona	29051502	1
Fagron	Cloridrato de metadona	339527	1
Fagron	Cloridrato de metadona	350571	1
Fagron	Cloridrato de metadona	4031517	1
Fagron	Cloridrato de metadona	414022-1-P	1
Fagron	Cloridrato de metadona	8081501	1
Fagron	Cloridrato de metadona	9041306	1
Fagron	Cloridrato de metadona	B03-3645508	1
Fagron	Cloridrato de metadona	F01-3764907	1
Fagron	Cloridrato de metadona	F04-3825003	1
Fagron	Cloridrato de metadona	F05-3705809	3
Fagron	Cloridrato de metadona	F05-3707509	3
Fagron	Cloridrato de metadona	F05-3714709	2
Fargon/Noweda	Cloridrato de metadona	18G02-B02-355989	1
Fargon	Cloridrato de metadona	16K01-B04-329937	1
Fgron GmbH & Co. KG	Cloridrato de metadona	18C01-B05-350571	1
Fiebig/	Cloridrato de metadona	67055	1
Fiebig/BLS	Cloridrato de metadona	70245	1
Fragon/ Gehe	Cloridrato de metadona	18G02-B02-355989	1
Fragon/Phönix	Cloridrato de metadona	18C01-B05-346737	1
Gatt-Koller	Cloridrato de metadona	1801702	1
Gehe/Noweda	Cloridrato de metadona	16135319	1
Gehe/P.W.Beyvers	Cloridrato de metadona	70245	4
gehe	Cloridrato de metadona	16135316	2
GEHE	Cloridrato de metadona	16135330	1
gehe	Cloridrato de metadona	17239502	1
Gehe	Cloridrato de metadona	17115-B02-339523	1
Gehe	Cloridrato de metadona	18132403	2
GEHE	Cloridrato de metadona	18132403	1
Gehe	Cloridrato de metadona	18G02-B02-355990	1
Gehe	Cloridrato de metadona	23001353007	1
Geilenkirchen	Cloridrato de metadona		1
Geilenkirchen	Cloridrato de metadona	16135309	1
GUMO	Cloridrato de metadona	19D09-B03-364513	1
Hedinger/ Sanacorp	Cloridrato de metadona	15215505	3
Jenne	Cloridrato de metadona	15B24-B02	1
Klosterring	Cloridrato de metadona	17I15-B02-343151	2
L30	Cloridrato de metadona	67055	6
L30	Cloridrato de metadona	70245	1
NOW	Cloridrato de metadona	23A25-F-02-384693	1
Noweda	Cloridrato de metadona	18132412	2
Noweda	Cloridrato de metadona	20a09f05370755	1
Noweda	Cloridrato de metadona	21003277024	1
Noweda	Cloridrato de metadona	23001353005	1
noweda	Cloridrato de metadona	3072001	1
Ph/Th Geiger GmbH	Cloridrato de metadona	70245	4
Phoenix	Cloridrato de metadona	15244715	1
Phoenix	Cloridrato de metadona	16125317	1
Phoenix	Cloridrato de metadona	191494003	1
Phoenix	Cloridrato de metadona	20D09F05	1
Phönix / Th.Greier 0...	Cloridrato de metadona	70245	1
Phönix	Cloridrato de metadona	14C24-B01-292860	1
Phönix	Cloridrato de metadona	16135309	1
PHÖNIX	Cloridrato de metadona	17239512	1
Phönix	Cloridrato de metadona	18C01-B05-350571	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Cloridrato de metadona	191494001	1
Phönix	Cloridrato de metadona	2100327706	1
Phönix	Cloridrato de metadona	67055	1
Phönix	Cloridrato de metadona	70245	2
Sana	Cloridrato de metadona	70617	1
Sanacorp	Cloridrato de metadona	12171913	1
Sanacorp	Cloridrato de metadona	12344806	2
Sanacorp	Cloridrato de metadona	18132408	1
Sanacorp	Cloridrato de metadona	18132417	2
Sanacorp	Cloridrato de metadona	70245	1
Saneca Pharmaceutica…	Cloridrato de metadona	19000787001	2
Saneca/Phoenix	Cloridrato de metadona	19149406	1
Sanocorp	Cloridrato de metadona	1608H002	1
Siegfried Ltd, Divis…	Cloridrato de metadona	15244712	1
Siegfried Ltd. Devis…	Cloridrato de metadona	17186104	1
Siegfried Ltd	Cloridrato de metadona	12B21-N03	1
Siegfried/Fiebig-BTM	Cloridrato de metadona	19D09-B03-364513	1
Th. Geyer	Cloridrato de metadona		1
Th. Geyer	Cloridrato de metadona	56(070245)	1
Th. Geyer	Cloridrato de metadona	67047	2
Th. Geyer	Cloridrato de metadona	67055	15
Th. Geyer	Cloridrato de metadona	70245	60
Th. Geyer	Cloridrato de metadona	70246	1
Th. Geyer	Cloridrato de metadona	70617	17
Th. Geyer	Cloridrato de metadona	70873	1
Th.Meyer GmbH	Cloridrato de metadona	70245	3
VDL;87,00EUR;08.09.14	Cloridrato de metadona	12344821	1

- 234 913 spectra from 1515 *Apo-Ident* customers from a total of 48 862 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de metadona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de metadona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	680	0	152 282
Type B	0	360	0	201 724
Type C	0	1121	33	234 913

The substance/substance group *Cloridrato de metadona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1176 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.9007 %)	97.1404 % (> 96.8804 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21170	21170	0,00	98,62
21172	21172	0,00	99,09
21174	21174	0,00	97,12
21176	21176	0,00	112,59
22417	22417	0,00	104,54
22428	22428	0,00	105,34
23485	23485	0,00	101,76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de metoclopramida monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21662-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de metoclopramida monoidratado; Metoclopramida, cloridrato monoidratado; Metoclopramidi hydrochloridum monohydricum

Special notes

When selecting the *Cloridrato de metoclopramida monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de metoclopramida monoidratado	6	3	5

Second-stage model

For differentiation of the substance/substance group *Cloridrato de metoclopramida monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de metoclopramida monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	108,21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de metoclopramida monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de metoclopramida monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de metoclopram…	14193102	21662	60	AR-15-FG-002889-01
Caelo	Cloridrato de metoclopram…	14193102	21746	60	20140725
Caelo	Cloridrato de metoclopram…	15421101	23234	40	20160226
Fagron	Cloridrato de metoclopram…	20G14-F05-374155	25584	40	20200826
Fagron	Cloridrato de metoclopram…	22A14-B04-227242	26544	40	20220318
Fagron	Cloridrato de metoclopram…	23J28-B01-231563	27040	40	20231119
Gatt-Koller	Cloridrato de metoclopram…	20170236	24410	40	20170724

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Cloridrato de metoclopramida monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Cloridrato de metoclopramida monoidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de metoclopram…	15421102	23718	40
Fagron	Cloridrato de metoclopram…	21F07-B08-213763	25863	50
Gatt-Koller	Cloridrato de metoclopram…	22J02736	26625	40
Fagron	Cloridrato de metoclopram…	22A14-B04-227242	26544SI†	20
Fagron	Cloridrato de metoclopram…	23J28-B01-231563	27040SI†	20
Gatt-Koller	Cloridrato de metoclopram…	22J02736	26625SI	20

- 201 894 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 23 spectra from 22 *Apo-Ident* customers from 5 batches from the substance/substance group *Cloridrato de metoclopramida monoidratado*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de metoclopram…	14193101	1
Caelo	Cloridrato de metoclopram…	15227001	18

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de metoclopram…	2818Q-01869	1
Caelo	Cloridrato de metoclopram…	3414U-018969	1
Caesar&loretz,Phoenix	Cloridrato de metoclopram…	14193101	1
Fragon/ Sanacorp	Cloridrato de metoclopram…	1/17M	1

- 236 044 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de metoclopramida monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de metoclopramida monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	190	0	201 894
Type C	0	23	0	236 044

The substance/substance group *Cloridrato de metoclopramida monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 73.9130 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21662	21662	0,00	211,03
21746	21662	5,25	211,15
23234	21662	7,78	213,27
24410	21662	6,73	212,75
25584	21662	16,15	214,92
26544	21662	15,12	217,84
27040	21662	16,50	215,37

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de midazolam**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20307-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de midazolam; Midazolam, cloridrato; Midazolami hydrochloridum

Special notes

When selecting the *Cloridrato de midazolam* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de midazolam	6	3	63

Second-stage model

For differentiation of the substance/substance group *Cloridrato de midazolam* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de midazolam* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hemissuccinato de doxilamina	124,76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de midazolam* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de midazolam*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de midazolam	12215811	21180	40	0914E-03538
Caelo	Cloridrato de midazolam	12215811	21180SI	60	0914E-03538
Caelo	Cloridrato de midazolam	15224602	22405	60	1516B-03538
Caelo	Cloridrato de midazolam	15224602	22405SI	60	1516B-03538
Fagron	Cloridrato de midazolam	13E22-N09	21182	40	0914F-03538
Fagron	Cloridrato de midazolam	13E22-N09	21182SI	60	0914F-03538
Fagron	Cloridrato de midazolam	14L23-B04-300245	22423	60	1516A-03538
Fagron	Cloridrato de midazolam	14L23-B04-300245	22423SI	60	1516A-03538
Fagron	Cloridrato de midazolam	15H04-B03-314396	23489	40	1917R-03538
Fagron	Cloridrato de midazolam	16C14-B12-332469	23925	40	0718E-03538
Fagron	Cloridrato de midazolam	16C14-B12-332469	23925SI	40	0718E-03538

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 560 spectra of 11 reference samples from the substance/substance group *Cloridrato de midazolam*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 402 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Cloridrato de midazolam*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de midazolam	15224611	23488	40
Fagron	Cloridrato de midazolam	15J07-B01-320717	23487	40
Fagron	Cloridrato de midazolam	18B28-B05-354856	24657	40
Caelo	Cloridrato de midazolam	15224611	23488SI	30
Fagron	Cloridrato de midazolam	15J07-B01-320717	23487SI	30
Fagron	Cloridrato de midazolam	15H04-B03-314396	23489SI†	30
Fagron	Cloridrato de midazolam	18B28-B05-354856	24657SI	40

- 201 834 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 157 spectra from 70 *Apo-Ident* customers from 65 batches from the substance/substance group *Cloridrato de midazolam*.

- Among them are spectra of independent samples from 63 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de midazolam	20002613005	1
	Cloridrato de midazolam	20I24-F01-374730	3
	Cloridrato de midazolam	21B03	1
	Cloridrato de midazolam	21B03-F50-384281	2
	Cloridrato de midazolam	24B16-F02-386032	1
Caelo	Cloridrato de midazolam	11184705	1
Caelo	Cloridrato de midazolam	143339009	1
Caelo	Cloridrato de midazolam	14339002	1
Caelo	Cloridrato de midazolam	14339009	1
Caelo	Cloridrato de midazolam	14339015	2
Caelo	Cloridrato de midazolam	15224603	1
Caelo	Cloridrato de midazolam	15224605	1
Caelo	Cloridrato de midazolam	15224607	1
Caelo	Cloridrato de midazolam	15224614	2
Caelo	Cloridrato de midazolam	15224616	3
Caelo	Cloridrato de midazolam	16290605	8
Caelo	Cloridrato de midazolam	17168001	1
Caelo	Cloridrato de midazolam	17168003	3
Caelo	Cloridrato de midazolam	17168005	1
Caelo	Cloridrato de midazolam	17168006	4
Caelo	Cloridrato de midazolam	17168007	3
Caelo	Cloridrato de midazolam	17168009	4
Caelo	Cloridrato de midazolam	17168011	4
Caelo	Cloridrato de midazolam	192213002	5
Caelo	Cloridrato de midazolam	20002613002	4
Caelo	Cloridrato de midazolam	20002613004	2
Caelo	Cloridrato de midazolam	2061508	1
Caelo	Cloridrato de midazolam	2100053006	1
Caelo	Cloridrato de midazolam	21003167002	2
Caelo	Cloridrato de midazolam	21003167008	1
Caelo	Cloridrato de midazolam	71680091	1
Caelo	Cloridrato de midazolam	83600116001	1
Caesar & Loretz GmbH...	Cloridrato de midazolam	21000038005	1
Caesar & Loretz GmbH...	Cloridrato de midazolam	2100003807	1
Caesar & Loretz GmbH...	Cloridrato de midazolam	20002613002	1
Caesar & Loretz GmbH...	Cloridrato de midazolam	20002613002	1
Caesar & Loretz GmbH...	Cloridrato de midazolam	21003167002	1
Caesar & Loretz GmbH...	Cloridrato de midazolam	21000038007	3
Caesar & Loretz GmbH...	Cloridrato de midazolam	17168007	3
Caesar & Loretz GmbH	Cloridrato de midazolam	17168006	1
Caesar & Loretz GmbH	Cloridrato de midazolam	20002613009	1
Caesar & Loretz GmbH	Cloridrato de midazolam	20002613010	1
Caesar & Loretz GmbH	Cloridrato de midazolam	21000038007	1
Caesar & Loretz GmbH	Cloridrato de midazolam	21000535006	1
Caesar & Loretz GmbH	Cloridrato de midazolam	21003167002	7
Caesar & Loretz GmbH	Cloridrato de midazolam	21003167004	1
Caesar & Loretz GmbH	Cloridrato de midazolam	21003167008	1
Cealo/ Noweda	Cloridrato de midazolam	17168006	1
Eurho/Phoenix	Cloridrato de midazolam	12L17-N10	1
Euro OTC	Cloridrato de midazolam	15224607	1
Fagron	Cloridrato de midazolam	11A31-NO1	1
Fagron	Cloridrato de midazolam	14H05-B08-297982	1
Fagron	Cloridrato de midazolam	15H04-B03-314396	9
Fagron	Cloridrato de midazolam	16C14-B12-332469	1
Fagron	Cloridrato de midazolam	17K21-B05-347538	2
Fagron	Cloridrato de midazolam	18B28-B05	1
Fagron	Cloridrato de midazolam	18B28-B05-354856	2
Fagron	Cloridrato de midazolam	18F19B02	1
Fagron	Cloridrato de midazolam	18F19-B02	1
Fagron	Cloridrato de midazolam	18F19B02-354857	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de midazolam	18F19-B02-354857	3
Fagron	Cloridrato de midazolam	19I25-F03-365483	1
Fagron	Cloridrato de midazolam	20124-F01-374730	1
Fagron	Cloridrato de midazolam	20D21-F02	1
Fagron	Cloridrato de midazolam	20D21-F02-370326	2
Fagron	Cloridrato de midazolam	20D21-F02-370327	1
Fagron	Cloridrato de midazolam	20F11-F04-374727	1
Fagron	Cloridrato de midazolam	20I24-F01	3
Fagron	Cloridrato de midazolam	20I24-F01-374728	7
Fagron	Cloridrato de midazolam	21B03-F50-384281	1
Fagron	Cloridrato de midazolam	30916	1
Fagron	Cloridrato de midazolam	400101	1
Fagron	Cloridrato de midazolam	940112	2
Fagron	Cloridrato de midazolam	9D27-N01	2
Fagron	Cloridrato de midazolam	F01-3747208	2
GEHE	Cloridrato de midazolam	16290605	1
JENNE	Cloridrato de midazolam	17168003	2
Noweda	Cloridrato de midazolam	17168011	1
Noweda	Cloridrato de midazolam	2100003805	1
Noweda	Cloridrato de midazolam	21000535006	1
Noweda	Cloridrato de midazolam	21003167002	1
Phönix	Cloridrato de midazolam	17168007	1
PHÖNIX	Cloridrato de midazolam	18B28-B05	1
Phönix	Cloridrato de midazolam	18F19-B02-354857	1
Sanacorp	Cloridrato de midazolam	16290605	1
Sanacorp	Cloridrato de midazolam	17168006	1

- 235 910 spectra from 1515 *Apo-Ident* customers from a total of 49 193 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de midazolam* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de midazolam* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	560	0	152 402
Type B	0	250	0	201 834
Type C	0	151	6	235 910

The substance/substance group *Cloridrato de midazolam* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9286 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	96.1783 % (> 94.2675 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21180	21180	0,00	260,00
21182	21182	0,00	258,92
22405	22405	0,00	260,18
22423	22423	0,00	241,68
23489	23489	0,00	257,17
23925	23925	0,00	172,36

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de morfina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21190-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de morfina; Morfina, cloridrato; Morphini hydrochloridum

Special notes

When selecting the *Cloridrato de morfina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de morfina	7	4	97

Second-stage model

For differentiation of the substance/substance group *Cloridrato de morfina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de morfina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	74,28	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de morfina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de morfina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de morfina	13125207	21190	40	0914E-01879
Caelo	Cloridrato de morfina	13125207	21190SI	60	0914E-01879
Caelo	Cloridrato de morfina	13349505	21192	40	0914F-01879
Caelo	Cloridrato de morfina	13349505	21192SI	60	0914F-01879
Caelo	Cloridrato de morfina	15439404	22409	60	1416R-01879
Caelo	Cloridrato de morfina	15439404	22409SI	60	1416R-01879
Caelo	Cloridrato de morfina	16184605	23490	40	1917S-01879
Fagron	Cloridrato de morfina	13G08-N04	21194	40	0914G-01879
Fagron	Cloridrato de morfina	13G08-N04	21194SI	60	0914G-01879
Fagron	Cloridrato de morfina	15I09-B08-312694	22421	60	1416Q-01879
Fagron	Cloridrato de morfina	15I09-B08-312694	22421SI	60	1416Q-01879
Th. Geyer	Cloridrato de morfina	67036	21196	40	0914H-01879
Th. Geyer	Cloridrato de morfina	67036	21196SI	60	0914H-01879

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 680 spectra of 13 reference samples from the substance/substance group *Cloridrato de morfina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 282 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 360 spectra of 9 reference samples from the substance/substance group *Cloridrato de morfina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de morfina	15439411	23491	40
Caelo	Cloridrato de morfina	18188607	24659	40
Fagron	Cloridrato de morfina	16D21-B02-322088	23492	40
Fagron	Cloridrato de morfina	17F22-B01-338170	24658	40
Caelo	Cloridrato de morfina	16184605	23490SI†	40
Caelo	Cloridrato de morfina	15439411	23491SI	40
Caelo	Cloridrato de morfina	18188607	24659SI	40
Fagron	Cloridrato de morfina	16D21-B02-322088	23492SI	40
Fagron	Cloridrato de morfina	17F22-B01-338170	24658SI	40

- 201 724 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 196 spectra from 97 *Apo-Ident* customers from 100 batches from the substance/substance group *Cloridrato de morfina*.

- Among them are spectra of independent samples from 95 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de morfina	20003757010	2
	Cloridrato de morfina	20003757015	1
	Cloridrato de morfina	21002337005	2
	Cloridrato de morfina	21002337009	1
	Cloridrato de morfina	23003282004	2
04655198	Cloridrato de morfina	2003757008	1
Caelo	Cloridrato de morfina		3
Caelo	Cloridrato de morfina	118188607	2
Caelo	Cloridrato de morfina	12104403	1
Caelo	Cloridrato de morfina	12104409	1
Caelo	Cloridrato de morfina	12318101	1
Caelo	Cloridrato de morfina	13081310	1
Caelo	Cloridrato de morfina	13125206	1
Caelo	Cloridrato de morfina	13125208	1
Caelo	Cloridrato de morfina	14055084	1
Caelo	Cloridrato de morfina	14081701	1
Caelo	Cloridrato de morfina	14238604	1
Caelo	Cloridrato de morfina	14238617	1
Caelo	Cloridrato de morfina	14238619	2
Caelo	Cloridrato de morfina	15199705	1
Caelo	Cloridrato de morfina	15199707	1
Caelo	Cloridrato de morfina	15199709	1
Caelo	Cloridrato de morfina	15199711	3
Caelo	Cloridrato de morfina	15199713	1
Caelo	Cloridrato de morfina	1543904	1
Caelo	Cloridrato de morfina	15439402	1
Caelo	Cloridrato de morfina	15439405	2
Caelo	Cloridrato de morfina	15439406	3
Caelo	Cloridrato de morfina	15439409	1
Caelo	Cloridrato de morfina	15439411	1
Caelo	Cloridrato de morfina	15439413	2
Caelo	Cloridrato de morfina	16184602	2
Caelo	Cloridrato de morfina	16184605	1
Caelo	Cloridrato de morfina	16184607	1
Caelo	Cloridrato de morfina	16184609	2
Caelo	Cloridrato de morfina	16184610	2
Caelo	Cloridrato de morfina	16184613	7
Caelo	Cloridrato de morfina	16184614	3
Caelo	Cloridrato de morfina	17258002	4
Caelo	Cloridrato de morfina	18188601	1
Caelo	Cloridrato de morfina	18188602	2
Caelo	Cloridrato de morfina	18188603	3
Caelo	Cloridrato de morfina	18188606	5
Caelo	Cloridrato de morfina	18188611	2
Caelo	Cloridrato de morfina	18188612	3
Caelo	Cloridrato de morfina	18188613	2
Caelo	Cloridrato de morfina	18188614	3
Caelo	Cloridrato de morfina	18188617	1
Caelo	Cloridrato de morfina	1818866	1
Caelo	Cloridrato de morfina	193085002	2
Caelo	Cloridrato de morfina	193085006	2
Caelo	Cloridrato de morfina	193085007	5
Caelo	Cloridrato de morfina	193085008	1
Caelo	Cloridrato de morfina	193085009	1
Caelo	Cloridrato de morfina	193085012	1
Caelo	Cloridrato de morfina	193085014	2
Caelo	Cloridrato de morfina	20001998002	2
Caelo	Cloridrato de morfina	20003757001	1
Caelo	Cloridrato de morfina	20003757003	2
Caelo	Cloridrato de morfina	20003757004	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de morfina	20003757008	1
Caelo	Cloridrato de morfina	20003757010	1
Caelo	Cloridrato de morfina	48188601	1
Caesar & Loretz GmbH...	Cloridrato de morfina	20003757008	1
Caesar & Loretz GmbH...	Cloridrato de morfina	193085002	1
Caesar & Loretz GmbH	Cloridrato de morfina	15199711	1
Caesar & Loretz GmbH	Cloridrato de morfina	15199711(1)	1
Caesar & Loretz GmbH	Cloridrato de morfina	15199711(2)	1
Caesar & Loretz GmbH	Cloridrato de morfina	15199712	1
Caesar & Loretz GmbH	Cloridrato de morfina	18188607	1
Caesar & Loretz GmbH	Cloridrato de morfina	18188610	2
Caesar & Loretz GmbH	Cloridrato de morfina	18188613	1
Caesar & Loretz GmbH	Cloridrato de morfina	18188614	3
Caesar & Loretz GmbH	Cloridrato de morfina	18188617	1
Caesar & Loretz GmbH	Cloridrato de morfina	193085003	1
Caesar & Loretz GmbH	Cloridrato de morfina	193085005	1
Caesar & Loretz GmbH	Cloridrato de morfina	193085006	2
Caesar & Loretz GmbH	Cloridrato de morfina	193085007	4
Caesar & Loretz GmbH	Cloridrato de morfina	20003757001	2
Caesar & Loretz GmbH	Cloridrato de morfina	20003757002	2
Caesar & Loretz GmbH	Cloridrato de morfina	20003757004	6
Caesar & Loretz GmbH	Cloridrato de morfina	20003757006	1
Fagron	Cloridrato de morfina	11A27-N04	1
Fagron	Cloridrato de morfina	12E10N04	1
Fagron	Cloridrato de morfina	12E10-N04	2
Fagron	Cloridrato de morfina	13D09-N04	1
Fagron	Cloridrato de morfina	13H22-N12	1
Fagron	Cloridrato de morfina	15/09-B08-312693	1
Fagron	Cloridrato de morfina	15A12-B04-303137	1
Fagron	Cloridrato de morfina	15I09-B08-312693	1
Fagron	Cloridrato de morfina	15J27_B01_316889	1
Fagron	Cloridrato de morfina	16D21-B02-322087	1
Fagron	Cloridrato de morfina	17C24-B03-334287	1
Fagron	Cloridrato de morfina	17F22-B01-338170	2
Fagron	Cloridrato de morfina	18B26-B04-351286	1
Fagron	Cloridrato de morfina	18F11-B03-357051	1
Fagron	Cloridrato de morfina	18F11-B03-361065	1
Fagron	Cloridrato de morfina	20E28-F06	1
Fagron	Cloridrato de morfina	20E28-F06-372132	3
Fagron	Cloridrato de morfina	B02-3220808	1
Jenne	Cloridrato de morfina	193085003	2
Jenne	Cloridrato de morfina	20001998001	1
Macfarlan Smith Limi...	Cloridrato de morfina	15199711	1
Noweda	Cloridrato de morfina	20003757001	1
Phoenix	Cloridrato de morfina	18F11-B03-357051	1
Phönix	Cloridrato de morfina	15I09-B08-312693	1
Phönix	Cloridrato de morfina	17258002	2
Phönix	Cloridrato de morfina	18188601	1
Sanacorp	Cloridrato de morfina	16184605	1
Sanacorp	Cloridrato de morfina	16184612	2
Sanacorp	Cloridrato de morfina	18188601	2
Sanacorp	Cloridrato de morfina	21002337005	1
Synop	Cloridrato de morfina	15I09-B08	1
Th. Geyer	Cloridrato de morfina	1415E-01879	1
Th. Geyer	Cloridrato de morfina	2615M-01879	1
Th. Geyer	Cloridrato de morfina	3518M-01879	1
Th. Geyer	Cloridrato de morfina	4117A-01879	1
Th. Geyer	Cloridrato de morfina	67036	5
Th. Geyer	Cloridrato de morfina	PH120087	1

- 235 871 spectra from 1515 *Apo-Ident* customers from a total of 49 158 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de morfina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de morfina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	680	0	152 282
Type B	0	360	0	201 724
Type C	0	196	0	235 871

The substance/substance group *Cloridrato de morfina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1176 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.9388 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21190	21190	0,00	154,48
21192	21192	0,00	145,01
21194	21194	0,00	157,70
21196	21196	0,00	158,43
22409	22409	0,00	164,37
22421	22421	0,00	164,80
23490	23490	0,00	158,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de nafazolina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20899-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de nafazolina; Nafazolina, cloridrato; Naphazolini hydrochloridum

Special notes

When selecting the *Cloridrato de nafazolina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de nafazolina	7	5	128

Second-stage model

For differentiation of the substance/substance group *Cloridrato de nafazolina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de nafazolina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de dexanfetamina	89,57	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de nafazolina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de nafazolina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de nafazolina	12375211	20899	40	20130108
Caelo	Cloridrato de nafazolina	12375211	21397	60	20130108
Caelo	Cloridrato de nafazolina	12375211	21398	60	20130108
Caelo	Cloridrato de nafazolina	181193	24498	40	20180504*
Euro OTC	Cloridrato de nafazolina	1407034-01	21623	60	AR-15-FG-007847-01
Euro OTC	Cloridrato de nafazolina	1506015	21859	60	20150727*
Euro OTC	Cloridrato de nafazolina	2003020	25260	40	20200706*
Euro OTC	Cloridrato de nafazolina	2008029	25304	40	20200908*
Fagron	Cloridrato de nafazolina	22K15-B02-223680	26449	40	20221129

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 9 reference samples from the substance/substance group *Cloridrato de nafazolina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Cloridrato de nafazolina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de nafazolina	161741	24496	40
Caelo	Cloridrato de nafazolina	21000140004	26620	40
Euro OTC	Cloridrato de nafazolina	1607041	22753	40
Euro OTC	Cloridrato de nafazolina	1704005	23385	40
Euro OTC	Cloridrato de nafazolina	1903006	24613	40
Caelo	Cloridrato de nafazolina	21000140004	26620SI	20
Fagron	Cloridrato de nafazolina	22K15-B02-223680	26449SI†	20

- 201 844 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 357 spectra from 255 *Apo-Ident* customers from 137 batches from the substance/substance group *Cloridrato de nafazolina*.

- Among them are spectra of independent samples from 128 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Cloridrato de nafazolina	20E29-B01-215556	1
	Cloridrato de nafazolina	22K15-B02-223680	3
	Cloridrato de nafazolina	22K15-B02-228533	2
apo-ident	Cloridrato de nafazolina	200802901	1
Caelo	Cloridrato de nafazolina	11081107	2
Caelo	Cloridrato de nafazolina	1206037	1
Caelo	Cloridrato de nafazolina	1216203	1
Caelo	Cloridrato de nafazolina	12176203	2
Caelo	Cloridrato de nafazolina	12375203	1
Caelo	Cloridrato de nafazolina	12375211	1
Caelo	Cloridrato de nafazolina	1307020-02	1
Caelo	Cloridrato de nafazolina	140703402	1
Caelo	Cloridrato de nafazolina	1506015-2	1
Caelo	Cloridrato de nafazolina	15071404	1
Caelo	Cloridrato de nafazolina	15223301	2
Caelo	Cloridrato de nafazolina	15223303	1
Caelo	Cloridrato de nafazolina	15J05-B05/171025NHC	1
Caelo	Cloridrato de nafazolina	160704101	1
Caelo	Cloridrato de nafazolina	1607041-01	1
Caelo	Cloridrato de nafazolina	16174101	5
Caelo	Cloridrato de nafazolina	1704005-02	2
Caelo	Cloridrato de nafazolina	1704005-03	1
Caelo	Cloridrato de nafazolina	17C02-805	1
Caelo	Cloridrato de nafazolina	17C02-B05-341579	1
Caelo	Cloridrato de nafazolina	18119302	10
Caelo	Cloridrato de nafazolina	18119311	1
Caelo	Cloridrato de nafazolina	18D09-B08-350950	2
Caelo	Cloridrato de nafazolina	18D09-B08-352462	1
Caelo	Cloridrato de nafazolina	18D09-B08-354882	1
Caelo	Cloridrato de nafazolina	1900054002	1
Caelo	Cloridrato de nafazolina	19000544002	6
Caelo	Cloridrato de nafazolina	19000544006	3
Caelo	Cloridrato de nafazolina	20002382001	1
Caelo	Cloridrato de nafazolina	20002392001	1
Caelo	Cloridrato de nafazolina	20E29-B01-196687	1
Caelo	Cloridrato de nafazolina	21000140004	6
Caelo	Cloridrato de nafazolina	2275310	1
Caelo	Cloridrato de nafazolina	732570001	1
Caelo	Cloridrato de nafazolina	9285103	2
Caesar & Loretz GmbH Og	Cloridrato de nafazolina	20002392001	1
Caesar & Loretz GmbH/Gehe	Cloridrato de nafazolina	18119302	1
Caesar & Loretz GmbH	Cloridrato de nafazolina	18119302	1
Caesar & Loretz GmbH	Cloridrato de nafazolina	19000544002	3
Caesar & Loretz GmbH	Cloridrato de nafazolina	20002392001	1
Caesar & Loretz GmbH	Cloridrato de nafazolina	20002392004	2
Caesar & Loretz GmbH	Cloridrato de nafazolina	21000140004	1
Caesar & Loretz GmbH	Cloridrato de nafazolina	21001702002	1
Caesar & Loretz/Engel	Cloridrato de nafazolina	18119302	2
Caesar / Ebert	Cloridrato de nafazolina	17C02-B05-341579	1
Caleo /Herba	Cloridrato de nafazolina	9285103	1
Eurho/Phoenix	Cloridrato de nafazolina	4413I-01885	1
EuRho/Phönix	Cloridrato de nafazolina	1704005-03	1
EuRho	Cloridrato de nafazolina	1114I-001885	1
Euro OTC	Cloridrato de nafazolina	1103031-02	1
Euro OTC	Cloridrato de nafazolina	113031-01	1
Euro OTC	Cloridrato de nafazolina	1206037-01	3
Euro OTC	Cloridrato de nafazolina	1206037-02	4
Euro OTC	Cloridrato de nafazolina	1307020-03	2
Euro OTC	Cloridrato de nafazolina	14070034-01	1
Euro OTC	Cloridrato de nafazolina	1407034-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de nafazolina	1407034-02	4
Euro OTC	Cloridrato de nafazolina	1407034-03	1
Euro OTC	Cloridrato de nafazolina	1506015-01	3
Euro OTC	Cloridrato de nafazolina	150601502	1
Euro OTC	Cloridrato de nafazolina	1506015-02	8
Euro OTC	Cloridrato de nafazolina	1607041	1
Euro OTC	Cloridrato de nafazolina	1607041-01	7
Euro OTC	Cloridrato de nafazolina	1704005-02	5
Euro OTC	Cloridrato de nafazolina	1704005-03	2
Euro OTC	Cloridrato de nafazolina	19030006-01	1
Euro OTC	Cloridrato de nafazolina	190300601	1
Euro OTC	Cloridrato de nafazolina	1903006-01	5
Euro OTC	Cloridrato de nafazolina	2003020-01	2
Euro OTC	Cloridrato de nafazolina	2008029-01	3
Euro OTC	Cloridrato de nafazolina	616620001	1
Euro/Sanacorp	Cloridrato de nafazolina	1704005-03	1
Fagron	Cloridrato de nafazolina	11/05-N02	1
Fagron	Cloridrato de nafazolina	1196687	1
Fagron	Cloridrato de nafazolina	11I05-N02	2
Fagron	Cloridrato de nafazolina	11J13-N08	1
Fagron	Cloridrato de nafazolina	11K25-N03	2
Fagron	Cloridrato de nafazolina	12K29-N01	1
Fagron	Cloridrato de nafazolina	12K29-N01o256/310	1
Fagron	Cloridrato de nafazolina	13/03-B03	1
Fagron	Cloridrato de nafazolina	13/03-B03-295105	2
Fagron	Cloridrato de nafazolina	13/03-B03305291	1
Fagron	Cloridrato de nafazolina	13/03-B03-305291	1
Fagron	Cloridrato de nafazolina	1303-B03	1
Fagron	Cloridrato de nafazolina	1303B03305291	1
Fagron	Cloridrato de nafazolina	13103-803-305291	1
Fagron	Cloridrato de nafazolina	13A07-N06	4
Fagron	Cloridrato de nafazolina	13C11N07	1
Fagron	Cloridrato de nafazolina	13C11-N07	5
Fagron	Cloridrato de nafazolina	13C11-NO7	1
Fagron	Cloridrato de nafazolina	13I03-B03	2
Fagron	Cloridrato de nafazolina	13I03-B03-295105	3
Fagron	Cloridrato de nafazolina	13I03-B03-305291	2
Fagron	Cloridrato de nafazolina	13k27-n04	1
Fagron	Cloridrato de nafazolina	13K27-N04	13
Fagron	Cloridrato de nafazolina	13l03-B03-295105	3
Fagron	Cloridrato de nafazolina	15J05-B05	2
Fagron	Cloridrato de nafazolina	15J05-B05-322527	4
Fagron	Cloridrato de nafazolina	15J05B05326850	1
Fagron	Cloridrato de nafazolina	15J05-B05-326850	3
Fagron	Cloridrato de nafazolina	15J05-B05-330834	3
Fagron	Cloridrato de nafazolina	17c02-b05	1
Fagron	Cloridrato de nafazolina	17C02-B05	4
Fagron	Cloridrato de nafazolina	17C02-B05-332933	5
Fagron	Cloridrato de nafazolina	17C02-B05-335113	1
Fagron	Cloridrato de nafazolina	17c02-b05-335313	1
Fagron	Cloridrato de nafazolina	17C02-B05-335313	5
Fagron	Cloridrato de nafazolina	17C02-B05-341579	5
Fagron	Cloridrato de nafazolina	17C02-B05-343566	4
Fagron	Cloridrato de nafazolina	17C02-B05-346657	2
Fagron	Cloridrato de nafazolina	17C02-B05-346657	1
Fagron	Cloridrato de nafazolina	1802201903	1
Fagron	Cloridrato de nafazolina	18D09	1
Fagron	Cloridrato de nafazolina	18D09-B08	2
Fagron	Cloridrato de nafazolina	18D09-B08-350950	3
Fagron	Cloridrato de nafazolina	18D09B08352462	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de nafazolina	18D09-B08-35462	1
Fagron	Cloridrato de nafazolina	18d09-b08-354882	1
Fagron	Cloridrato de nafazolina	18D09-B08-354882	7
Fagron	Cloridrato de nafazolina	18D09-B08-52462	1
Fagron	Cloridrato de nafazolina	18D09-BO8-352462	1
Fagron	Cloridrato de nafazolina	19D03B02362717	1
Fagron	Cloridrato de nafazolina	19D03-B02-362717	5
Fagron	Cloridrato de nafazolina	20E29-801-196687	1
Fagron	Cloridrato de nafazolina	20E29-B01_196687	1
Fagron	Cloridrato de nafazolina	20e29b01196687	1
Fagron	Cloridrato de nafazolina	20E29B01196687	1
Fagron	Cloridrato de nafazolina	20E29-B01-196687	24
Fagron	Cloridrato de nafazolina	20E29-BO1-196687	1
Fagron	Cloridrato de nafazolina	20E801196687	1
Fagron	Cloridrato de nafazolina	20E29B01196687	1
Fagron	Cloridrato de nafazolina	4309I-01885	1
Fagron	Cloridrato de nafazolina	4509E-01885	2
Fagron	Cloridrato de nafazolina	60494000113K27-N04	1
Fagron	Cloridrato de nafazolina	672530001	2
Fagron	Cloridrato de nafazolina	7001260012	1
Fagron	Cloridrato de nafazolina	700126-0012	1
Fagron	Cloridrato de nafazolina	706230001	3
Fagron	Cloridrato de nafazolina	708360002	1
Fagron	Cloridrato de nafazolina	9A09-N28	1
Fagron	Cloridrato de nafazolina	b01-1966807	1
Fagron	Cloridrato de nafazolina	B01-1966807	6
Fagron	Cloridrato de nafazolina	NPZ3020007	2
Fagron	Cloridrato de nafazolina	NPZ3O20007	2
Fargon/ Phönix	Cloridrato de nafazolina	20E29-B01-196687	1
Fargon/Apo.am Park	Cloridrato de nafazolina	539580002	1
Fargon/Noweda	Cloridrato de nafazolina	17C02-B05-346657	1
Fargon	Cloridrato de nafazolina	13/03-B03-295105	1
Fargron/Noweda	Cloridrato de nafazolina	20E29-B01-196687	1
Fragon GmbH/ Noweda	Cloridrato de nafazolina	15J05-B05-326850	1
Gatt-Koller	Cloridrato de nafazolina	1803834	1
Gehe/EuRho	Cloridrato de nafazolina	2008029-01	1
Gehe/EuRo	Cloridrato de nafazolina	1607041-01	1
Gehe	Cloridrato de nafazolina	17C02-B05-335313	1
Gehe	Cloridrato de nafazolina	19D03-B02-362717	2
Gehe	Cloridrato de nafazolina	20E29-B01-196687	1
Geilenkirchen	Cloridrato de nafazolina	18D09-B08-354882	1
Herberata Arzneimittel	Cloridrato de nafazolina	15223303I-02082016	1
Jenne	Cloridrato de nafazolina	2008029-01	1
LOBA / Gehe	Cloridrato de nafazolina	1903006-01	1
Loba / Gehe	Cloridrato de nafazolina	588710001	1
Nachprüfung	Cloridrato de nafazolina	3318E-1885	1
Noweda	Cloridrato de nafazolina	1704005-02	1
Noweda	Cloridrato de nafazolina	1903006-01	1
Noweda	Cloridrato de nafazolina	2003020-01	1
Noweda	Cloridrato de nafazolina	2008029-01	1
Noweda-Fragon	Cloridrato de nafazolina	1303B03305291	1
Otto Geilenkirchen	Cloridrato de nafazolina	22K15-B02-223680	1
Phoenix	Cloridrato de nafazolina	20E29-E01-196687	1
Phoenix	Cloridrato de nafazolina	22K15-B02-223680	1
Phonix	Cloridrato de nafazolina	1704005-02	1
Phönix	Cloridrato de nafazolina	1704005-02	2
Phönix	Cloridrato de nafazolina	586550002	1
Phönix	Cloridrato de nafazolina	B01-1966807	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 710 spectra from 1515 *Apo-Ident* customers from a total of 49 121 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de nafazolina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de nafazolina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	240	0	201 844
Type C	0	357	0	235 710

The substance/substance group *Cloridrato de nafazolina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.3193 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20899	21859	16,01	157,87
21397	21859	4,29	164,62
21398	21859	4,45	160,45
21623	21623	0,00	161,84
21859	21859	0,00	163,67
24498	24498	0,00	154,89
25260	25260	0,00	133,55
25304	25304	0,00	131,09
26449	25260	6,96	135,48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de naloxona di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20957-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de naloxona di-hidratado; Naloxona, cloridrato di-hidratado; Naloxoni hydrochloridum dihydricum

Special notes

When selecting the *Cloridrato de naloxona di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de naloxona di-hidratado	9	8	43

Second-stage model

For differentiation of the substance/substance group *Cloridrato de naloxona di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de naloxona di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	73,02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de naloxona di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de naloxona di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Cloridrato de naloxona di…	AP13501078IIN	22811	40	20160429
Audor Pharma	Cloridrato de naloxona di…	AP1547I022-1N	24707	40	20180629
Caelo	Cloridrato de naloxona di…	163577	23039	40	20170306*
Caelo	Cloridrato de naloxona di…	170441	23862	40	20170306*
Caelo	Cloridrato de naloxona di…	20001602	25447	40	20200604*
Euro OTC	Cloridrato de naloxona di…	2103008	25682	40	20210430*
Fagron	Cloridrato de naloxona di…	13D22-N07	20957	40	1402059
Fagron	Cloridrato de naloxona di…	13L12-B03	21271	40	20140113
Fagron	Cloridrato de naloxona di…	21J11-B10-216368	26175	40	20211118
Fagron	Cloridrato de naloxona di…	21J11-B10-216368	26175SI	40	20211118

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Cloridrato de naloxona di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 370 spectra of 10 reference samples from the substance/substance group *Cloridrato de naloxona di-hidratado*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de naloxona di…	15322517	22828	40
Caelo	Cloridrato de naloxona di…	190088	24537	40
Caelo	Cloridrato de naloxona di…	21000770009	26316	30
Caelo	Cloridrato de naloxona di…	22001102	27112	40
Euro OTC	Cloridrato de naloxona di…	2002011	25134	40
Euro OTC	Cloridrato de naloxona di…	2003062	25246	40
Euro OTC	Cloridrato de naloxona di…	2206005	26220	40
Euro OTC	Cloridrato de naloxona di…	2402028	27274	40
Caelo	Cloridrato de naloxona di…	21000770009	26316SI	20
Euro OTC	Cloridrato de naloxona di…	2206005	26220SI	40

- 201 714 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 75 spectra from 27 *Apo-Ident* customers from 44 batches from the substance/substance group *Cloridrato de naloxona di-hidratado*.

- Among them are spectra of independent samples from 43 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de naloxona di…	22001102004	1
	Cloridrato de naloxona di…	22001102008	1
Audor Pharma	Cloridrato de naloxona di…	AP13501078N	1
Audor Pharma	Cloridrato de naloxona di…	AP1547I022N	1
Caelo	Cloridrato de naloxona di…	15322501	1
Caelo	Cloridrato de naloxona di…	15322504	2
Caelo	Cloridrato de naloxona di…	15322517	1
Caelo	Cloridrato de naloxona di…	17044103	2
Caelo	Cloridrato de naloxona di…	18134202	3
Caelo	Cloridrato de naloxona di…	19008803	1
Caelo	Cloridrato de naloxona di…	20001602003	1
Caelo	Cloridrato de naloxona di…	2001602303	1
Caesar & Loretz GmbH	Cloridrato de naloxona di…	19008803	2
Caesar & Loretz GmbH	Cloridrato de naloxona di…	20001602003	1
Euro OTC	Cloridrato de naloxona di…	2002011-01	1
Euro OTC	Cloridrato de naloxona di…	2003062-01	1
Fagron	Cloridrato de naloxona di…	11/23-N01	1
Fagron	Cloridrato de naloxona di…	12-00071	2
Fagron	Cloridrato de naloxona di…	12G19-N02	2
Fagron	Cloridrato de naloxona di…	12G19-NO2	1
Fagron	Cloridrato de naloxona di…	13-00660	1
Fagron	Cloridrato de naloxona di…	1350I078	1
Fagron	Cloridrato de naloxona di…	13L12-B03-289511	1
Fagron	Cloridrato de naloxona di…	14A28-B33-296076	1
Fagron	Cloridrato de naloxona di…	14F20-B02-296077	1
Fagron	Cloridrato de naloxona di…	15B06-B02-304420	2
Fagron	Cloridrato de naloxona di…	15B06-B02-304421	1
Fagron	Cloridrato de naloxona di…	15E28-B01-308324	5
Fagron	Cloridrato de naloxona di…	15H04-B09	3
Fagron	Cloridrato de naloxona di…	15H04-B09-314068	5
Fagron	Cloridrato de naloxona di…	15K11-B05_319571	1
Fagron	Cloridrato de naloxona di…	15K11-B05-319571	4
Fagron	Cloridrato de naloxona di…	18-00116	1
Fagron	Cloridrato de naloxona di…	18452304	1
Fagron	Cloridrato de naloxona di…	18C30-B04-349699	2
Fagron	Cloridrato de naloxona di…	18K20-B05-356947	4
Fagron	Cloridrato de naloxona di…	18K20-B05-356948	1
Fagron	Cloridrato de naloxona di…	19J22-F03	1
Fagron	Cloridrato de naloxona di…	19J22-F03-367715	2
Fagron	Cloridrato de naloxona di…	19J22-F03-367716	1
Fagron	Cloridrato de naloxona di…	19J22-F03-368419	1
Fagron	Cloridrato de naloxona di…	19J22-FO3-367715	1
Fagron	Cloridrato de naloxona di…	20F15-01-372577	1
Fagron	Cloridrato de naloxona di…	20F15-F01-372577	2
Fagron	Cloridrato de naloxona di…	20f15-f01-372581	2
Fagron	Cloridrato de naloxona di…	20F15-F01-372581	2

- 235 992 spectra from 1515 *Apo-Ident* customers from a total of 49 214 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de naloxona di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de naloxona di-hidratado* and it was evaluated how many matches (positive) and rejections (negative)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	370	0	201 714
Type C	0	75	0	235 992

The substance/substance group *Cloridrato de naloxona di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3784 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20957	20957	0,00	89,68
21271	20957	11,09	86,01
22811	20957	21,25	92,34
23039	23039	0,00	93,62
23862	23862	0,00	92,62
24707	23039	20,77	96,04
25447	25447	0,00	81,46
25682	25682	0,00	88,69
26175	25682	22,31	86,36

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de naltrexona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006052-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de naltrexona; Naltrexona, cloridrato; Naltrexoni hydrochloridum

Special notes

When selecting the *Cloridrato de naltrexona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de naltrexona	5	1	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de naltrexona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de naltrexona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de naloxona di-hidratado	68,69	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de naltrexona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de naltrexona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de naltrexona	2212013	26512	30	20221222*
Euro OTC	Cloridrato de naltrexona	2212013	26512SI	20	20221222*
Euro OTC	Cloridrato de naltrexona	2307013	26864	40	20230821*
Euro OTC	Cloridrato de naltrexona	2307013	26864SI	20	20230821*
Euro OTC	Cloridrato de naltrexona	2401025	27343	40	20240812*
Euro OTC	Cloridrato de naltrexona	2401025	27343SI	20	20240812*
Fagron	Cloridrato de naltrexona	22G14-B03-226174	26454	40	240401868
Fagron	Cloridrato de naltrexona	22G14-B03-226174	26454SI	20	240401868
Fagron	Cloridrato de naltrexona	24A19-B02-237101	27183	40	240704587

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 270 spectra of 9 reference samples from the substance/substance group *Cloridrato de naltrexona*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 692 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Cloridrato de naltrexona*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de naltrexona	23E16-B06-232752	26979	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de naltrexona*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de naltrexona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de naltrexona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de naltrexona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26454	26454	0,00	236,09
26512	26512	0,00	257,24
26864	26864	0,00	115,53
27183	27183	0,00	244,92
27343	27343	0,00	179,28

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de noscapina monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006312-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de noscapina monoidratado; Noscapina, cloridrato monoidratado; Noscapini hydrochloridum hydricum

Special notes

When selecting the *Cloridrato de noscapina monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de noscapina monoidratado	3	1	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de noscapina monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de noscapina monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloreto de metacolina	114,82	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de noscapina monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de noscapina monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de noscapina m…	23F20-B11-231036	26899	40	240603357
Fagron	Cloridrato de noscapina m…	24C23-B04-235324	27379	40	20240426
Gatt-Koller	Cloridrato de noscapina m…	23J00299	26675	35	240401847

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 115 spectra of 3 reference samples from the substance/substance group *Cloridrato de noscapina monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 847 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 4 reference samples from the substance/substance group *Cloridrato de noscapina monoidratado*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Gatt-Koller	Cloridrato de noscapina m...	22J02175	26676	40
Fagron	Cloridrato de noscapina m...	23F20-B11-231036	26899SI†	20
Gatt-Koller	Cloridrato de noscapina m...	23J00299	26675SI†	20
Gatt-Koller	Cloridrato de noscapina m...	22J02175	26676SI	20

- 201 984 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de noscapina monoidratado*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de noscapina monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de noscapina monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	115	0	152 847
Type B	0	100	0	201 984
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de noscapina monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.7826 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26675	26675	0,00	205,67
26899	26899	0,00	188,59
27379	26899	77,98	201,39

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de ornitina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20389-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de ornitina; Ornithini hydrochloridum; Ornitina, cloridrato

Special notes

When selecting the *Cloridrato de ornitina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de ornitina	8	10	15

Second-stage model

For differentiation of the substance/substance group *Cloridrato de ornitina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de ornitina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	86,39	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de ornitina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de ornitina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de ornitina	1307028-01	21622	120	20130813
Euro OTC	Cloridrato de ornitina	1605011	22573	40	20160601*
Euro OTC	Cloridrato de ornitina	1612009	22923	40	20170113*
Euro OTC	Cloridrato de ornitina	2001004	25084	40	20200123*
Euro OTC	Cloridrato de ornitina	2004018	25271	40	20200731*
Euro OTC	Cloridrato de ornitina	2305021	26751	40	20230616*
Euro OTC	Cloridrato de ornitina	2305021	26751SI	20	20230616*
Euro OTC	Cloridrato de ornitina	2408003	27391	40	20241029*
Fagron	Cloridrato de ornitina	13A03-N05	20967	40	1403094

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 9 reference samples from the substance/substance group *Cloridrato de ornitina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 12 reference samples from the substance/substance group *Cloridrato de ornitina*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de ornitina	1612009-01	23009	40
Euro OTC	Cloridrato de ornitina	1704006	23159	40
Euro OTC	Cloridrato de ornitina	1803018	24085	40
Euro OTC	Cloridrato de ornitina	1906015	24810	40
Euro OTC	Cloridrato de ornitina	2101021	25547	40
Euro OTC	Cloridrato de ornitina	2103016	25598	40
Euro OTC	Cloridrato de ornitina	2107018	25764	50
Euro OTC	Cloridrato de ornitina	2201012	26042	40
Euro OTC	Cloridrato de ornitina	2301046	26572	40
Euro OTC	Cloridrato de ornitina	2409011	27392	40
Euro OTC	Cloridrato de ornitina	2201012	26042SI	10
Euro OTC	Cloridrato de ornitina	2301046	26572SI	20

- 201 644 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 5 *Apo-Ident* customers from 16 batches from the substance/substance group *Cloridrato de ornitina*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de ornitina	1014I-03475	1
Euro OTC	Cloridrato de ornitina	1704006-01	1
Euro OTC	Cloridrato de ornitina	1906015-01	1
Euro OTC	Cloridrato de ornitina	2001004-01	1
Euro OTC	Cloridrato de ornitina	2004018-01	9
Euro OTC	Cloridrato de ornitina	2101021-01	1
Euro OTC	Cloridrato de ornitina	2103016-01	1
Euro OTC	Cloridrato de ornitina	2107018-01	1
Euro OTC	Cloridrato de ornitina	2201012-01	1
Euro OTC	Cloridrato de ornitina	2201012-02	1
Euro OTC	Cloridrato de ornitina	315E-03475	1
Euro OTC	Cloridrato de ornitina	4712A-03475	1
Euro OTC	Cloridrato de ornitina	516Q-03475	1
Euro OTC	Cloridrato de ornitina	5217M-03475	1
Fagron	Cloridrato de ornitina	13A03-N05	1
Fagron	Cloridrato de ornitina	15A13-B03	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de ornitina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de ornitina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	440	0	201 644
Type C	0	24	0	236 043

The substance/substance group *Cloridrato de ornitina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 75.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20967	20967	0,00	201,14
21622	22573	3,25	200,64
22573	22573	0,00	200,75
22923	22923	0,00	200,93
25084	25084	0,00	201,99
25271	25271	0,00	200,24
26751	26751	0,00	201,13
27391	27391	0,00	202,88

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de oxibuprocaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20958-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de oxibuprocaína; Oxibuprocaína, cloridrato; Oxybuprocaini hydrochloridum

Special notes

When selecting the *Cloridrato de oxibuprocaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de oxibuprocaína	6	3	17

Second-stage model

For differentiation of the substance/substance group *Cloridrato de oxibuprocaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de oxibuprocaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	111,55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de oxibuprocaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de oxibuprocaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de oxibuprocaína	13D16-N12	20958	40	1402060
Fagron	Cloridrato de oxibuprocaína	13J24-B07-295015	21799	60	AR-15-FG-014812-02
Fagron	Cloridrato de oxibuprocaína	13J24-B07-295015	21799SI	60	AR-15-FG-014812-02
Fagron	Cloridrato de oxibuprocaína	15A26-B07-306787	21922	60	20150203
Fagron	Cloridrato de oxibuprocaína	15A26-B07-306787	21922SI	60	20150203
Fagron	Cloridrato de oxibuprocaína	16L05-B06-334330	23719	40	20170113
Fagron	Cloridrato de oxibuprocaína	16L05-B06-334330	23720	40	20170113
Fagron	Cloridrato de oxibuprocaína	17G21-B03-338576	23745	40	20170823
Fagron	Cloridrato de oxibuprocaína	16L05-B06-334330	23752	40	20170113
Fagron	Cloridrato de oxibuprocaína	19K04-B04-195510	25581	40	20191114

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 10 reference samples from the substance/substance group *Cloridrato de oxibuprocaína*. These samples are listed above in the *calibration samples* section. The reference

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

samples come from 6 different batches.

- 152 482 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 4 reference samples from the substance/substance group *Cloridrato de oxibuprocaína*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cloridrato de oxibuprocaína	18F20-B02-355633	24580	40
Fagron	Cloridrato de oxibuprocaína	20B13-B01-197691	25744	50
Fagron	Cloridrato de oxibuprocaína	20I03-B06-202527	25940	40
Fagron	Cloridrato de oxibuprocaína	20I03-B06-202527	25940SI	40

- 201 914 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 12 *Apo-Ident* customers from 18 batches from the substance/substance group *Cloridrato de oxibuprocaína*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de oxibuprocaína	14G21B02300384	1
Fagron	Cloridrato de oxibuprocaína	12L19N01	1
Fagron	Cloridrato de oxibuprocaína	13C01-N01	4
Fagron	Cloridrato de oxibuprocaína	13h13-n05	2
Fagron	Cloridrato de oxibuprocaína	13J24B07295015	1
Fagron	Cloridrato de oxibuprocaína	15A26-B07	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de oxibuprocaína	16L05-B06	1
Fagron	Cloridrato de oxibuprocaína	16L05-B06-332495	1
Fagron	Cloridrato de oxibuprocaína	18F20-B02-351233	1
Fagron	Cloridrato de oxibuprocaína	18F20-B02-355633	1
Fagron	Cloridrato de oxibuprocaína	19K04-B04-195510	1
Fagron	Cloridrato de oxibuprocaína	19K04-B04-195511	1
Fagron	Cloridrato de oxibuprocaína	20B13-B01-197691	2
Fagron	Cloridrato de oxibuprocaína	20I03-B06-202527	2
Fagron	Cloridrato de oxibuprocaína	3613N-07321	1
Fagron	Cloridrato de oxibuprocaína	4612M-03639	1
Klenk	Cloridrato de oxibuprocaína	3613M-07321	1
Phönix	Cloridrato de oxibuprocaína	16L05-B06-329642	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de oxibuprocaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de oxibuprocaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	170	0	201 914
Type C	0	23	1	236 043

The substance/substance group *Cloridrato de oxibuprocaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	95.8333 % (> 83.3333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20958	20958	0,00	142,03
21799	21799	0,00	120,27
21922	21799	11,44	136,28
23719	21799	17,80	142,63
23720	21799	15,71	140,47
23745	21799	18,06	142,45
23752	21799	20,96	144,80
25581	21799	16,40	140,11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de oxibutinina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20565-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de oxibutinina; Oxibutinina, cloridrato; Oxybutynini hydrochloridum

Special notes

When selecting the *Cloridrato de oxibutinina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de oxibutinina	6	8	79

Second-stage model

For differentiation of the substance/substance group *Cloridrato de oxibutinina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de oxibutinina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	116,40	–
⋮	⋮	⋮
Prednicarbato	>50	66,94
Levocarnitina	>50	96,10
Acetato de ciproterona	>50	110,21
Capsaicina	>50	110,53
Citrato de sódio	>50	145,62
Tetracaína	>50	204,28
Acetato de noretisterona	>50	268,17
Alfaestradiol	>50	294,99
Cloridrato de amitriptilina	>50	316,58
Cloridrato de quinina di-hidratado	>50	326,78
Valina	>50	438,10
Piridoxal-5-fosfato	>50	440,29
Metoxisaleno	>50	468,83
Heparina sódica	>50	548,50
Cloridrato de ciprofloxacina	>50	554,59
Triclosan	>50	1588,05
Amifampridina	>50	1875,42
Sacarose	>50	1955,66

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de oxibutinina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de oxibutinina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de oxibutinina	2005030	25351	40	20200911*
Euro OTC	Cloridrato de oxibutinina	2010024	25457	40	20201201*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cloridrato de oxibutinina	13H26-B03-290572	21543	60	AR-15-FG-002173-01
Fagron	Cloridrato de oxibutinina	14A29-B09-293841	21704	45	20140227
Fagron	Cloridrato de oxibutinina	14I16-B03-312059	22732	40	20141007
Fagron	Cloridrato de oxibutinina	18K22-B01-359482	25059	40	20181217

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 265 spectra of 6 reference samples from the substance/substance group *Cloridrato de oxibutinina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 697 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 11 reference samples from the substance/substance group *Cloridrato de oxibutinina*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de oxibutinina	2205010	26189	40
Euro OTC	Cloridrato de oxibutinina	2301024	26578	40
Euro OTC	Cloridrato de oxibutinina	2310011	27062	40
Euro OTC	Cloridrato de oxibutinina	2403009	27211	40
Fagron	Cloridrato de oxibutinina	12D24-N07	20565	40
Fagron	Cloridrato de oxibutinina	16A18-B02-321181	23268	40
Fagron	Cloridrato de oxibutinina	18A12-B03-344347	23995	40
Fagron	Cloridrato de oxibutinina	21H27-B01-220138	26288	40
Euro OTC	Cloridrato de oxibutinina	2205010	26189SI	20
Euro OTC	Cloridrato de oxibutinina	2301024	26578SI	20
Fagron	Cloridrato de oxibutinina	21H27-B01-220138	26288SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 704 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 199 spectra from 66 *Apo-Ident* customers from 84 batches from the substance/substance group *Cloridrato de oxibutinina*.

- Among them are spectra of independent samples from 79 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de oxibutinina	21H27-B01-224479	2
	Cloridrato de oxibutinina	21H27-B01-227285	1
	Cloridrato de oxibutinina	B0122013008	1
	Cloridrato de oxibutinina	CC0100362	1
Audor Pharma	Cloridrato de oxibutinina		3
Audor Pharma	Cloridrato de oxibutinina	APOH/043/2017-2018	2
Audor Pharma	Cloridrato de oxibutinina	APOH/067/2018-2019	2
Audor Pharma	Cloridrato de oxibutinina	APOH0122017201810B	2
Audor Pharma	Cloridrato de oxibutinina	APOH0122017-2018-10B	1
Caelo	Cloridrato de oxibutinina	129099	1
Caelo	Cloridrato de oxibutinina	14A29-B09-307322	4
Caelo	Cloridrato de oxibutinina	15F05_B03_315221	5
Caelo	Cloridrato de oxibutinina	15F05-B03-318524	4
Caelo	Cloridrato de oxibutinina	16/23-B03-328916	1
Caelo	Cloridrato de oxibutinina	16/23-B03-333371	3
Caelo	Cloridrato de oxibutinina	16A18_B02_321181	2
Caelo	Cloridrato de oxibutinina	16A18-B02-321181	3
Caelo	Cloridrato de oxibutinina	16A18-B02-326183	1
Caelo	Cloridrato de oxibutinina	16I23-B03-328916	1
Caelo	Cloridrato de oxibutinina	18A12-B03	2
Caelo	Cloridrato de oxibutinina	18A12-B03-344348	1
Caelo	Cloridrato de oxibutinina	18A12-B03-344350	1
Caelo	Cloridrato de oxibutinina	18A12-Bo3-344350	1
Euro OTC	Cloridrato de oxibutinina	2010024-01	4
Euro OTC	Cloridrato de oxibutinina	2010024-02	1
Fagro/Sanacorp	Cloridrato de oxibutinina	16/23-B03-32891613	1
Fagro/Sanacorp	Cloridrato de oxibutinina	16A18-B02-326183	1
Fagron	Cloridrato de oxibutinina	127979	2
Fagron	Cloridrato de oxibutinina	129099	1
Fagron	Cloridrato de oxibutinina	130563	1
Fagron	Cloridrato de oxibutinina	13H26-B03	1
Fagron	Cloridrato de oxibutinina	13H26-B03-287325	1
Fagron	Cloridrato de oxibutinina	14/16_B03_300207	1
Fagron	Cloridrato de oxibutinina	14/16-B03-300207	5
Fagron	Cloridrato de oxibutinina	14/16-B03-300209	1
Fagron	Cloridrato de oxibutinina	14A29_B09_307322	2
Fagron	Cloridrato de oxibutinina	14a29-b09-307322	2
Fagron	Cloridrato de oxibutinina	14A29-B09-307322	1
Fagron	Cloridrato de oxibutinina	14I16-B03	1
Fagron	Cloridrato de oxibutinina	14I16-B03-300207	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de oxibutinina	15F05-b03-315220	1
Fagron	Cloridrato de oxibutinina	15F05-B03-315221	6
Fagron	Cloridrato de oxibutinina	15F05-B03-318524	1
Fagron	Cloridrato de oxibutinina	16/23-b03-333371	1
Fagron	Cloridrato de oxibutinina	1607080	1
Fagron	Cloridrato de oxibutinina	16A18-B02-322538	3
Fagron	Cloridrato de oxibutinina	16A18-B02-326183	3
Fagron	Cloridrato de oxibutinina	16I23-B03-328916	3
Fagron	Cloridrato de oxibutinina	16I23-B03-329448	1
Fagron	Cloridrato de oxibutinina	16I23-B03-333371	2
Fagron	Cloridrato de oxibutinina	16l23-b03-328916	1
Fagron	Cloridrato de oxibutinina	170925O/16I23-B03-33	1
Fagron	Cloridrato de oxibutinina	18A12-B03	2
Fagron	Cloridrato de oxibutinina	18A12-B03-344347	1
Fagron	Cloridrato de oxibutinina	18A12-B03-344348	6
Fagron	Cloridrato de oxibutinina	18A12-B03-344350	1
Fagron	Cloridrato de oxibutinina	18A12-B03-345554	1
Fagron	Cloridrato de oxibutinina	18A12-B03-346964	4
Fagron	Cloridrato de oxibutinina	18A12-B03-347807	1
Fagron	Cloridrato de oxibutinina	18A12B03349624	1
Fagron	Cloridrato de oxibutinina	18A12-B03-349624	3
Fagron	Cloridrato de oxibutinina	18A12-B03-350471	3
Fagron	Cloridrato de oxibutinina	18A12-B03-351262	2
Fagron	Cloridrato de oxibutinina	18A12B03352129	1
Fagron	Cloridrato de oxibutinina	18A12-B03-353049	1
Fagron	Cloridrato de oxibutinina	18A23-B03-351262	1
Fagron	Cloridrato de oxibutinina	18K22-B01	2
Fagron	Cloridrato de oxibutinina	18K22-B01-358358	2
Fagron	Cloridrato de oxibutinina	18K22-B01-359482	7
Fagron	Cloridrato de oxibutinina	18K22-B01-363434	1
Fagron	Cloridrato de oxibutinina	18K22-B01-363953	2
Fagron	Cloridrato de oxibutinina	20K100-F04-375776	1
Fagron	Cloridrato de oxibutinina	20K10-F04	1
Fagron	Cloridrato de oxibutinina	20K10-F04	1
Fagron	Cloridrato de oxibutinina	20K10-F04-3757706	2
Fagron	Cloridrato de oxibutinina	20K10-F04-375776	5
Fagron	Cloridrato de oxibutinina	20K10-F04-375777	13
Fagron	Cloridrato de oxibutinina	21G01-F05-379447	9
Fagron	Cloridrato de oxibutinina	21H27-B01-2164002	1
Fagron	Cloridrato de oxibutinina	21H27-B01-218125	3
Fagron	Cloridrato de oxibutinina	21H27-B01-220138	1
Fagron	Cloridrato de oxibutinina	22032E005	1
Fagron	Cloridrato de oxibutinina	22032F004	5
Fagron	Cloridrato de oxibutinina	4375777	1
Fagron	Cloridrato de oxibutinina	5-37944007	1
Fagron	Cloridrato de oxibutinina	F04-3757706	2
Fagron	Cloridrato de oxibutinina	F04-3757707	1
Fagron	Cloridrato de oxibutinina	F04-375776	1
Fagron	Cloridrato de oxibutinina	F05-379449	1
Fagron	Cloridrato de oxibutinina	LCA0100105	1
Fagron	Cloridrato de oxibutinina	OH/044/2020-2021	1
Krieger	Cloridrato de oxibutinina	F04-3757707	1
Noweda	Cloridrato de oxibutinina	18A12-B03-347807	1
Noweda	Cloridrato de oxibutinina	18A12-B03-351262	1
Phoenix	Cloridrato de oxibutinina	16/23-BO3-328916	1
Phoenix	Cloridrato de oxibutinina	18A12-B03-346964	1
Phoenix	Cloridrato de oxibutinina	22032E005	2
Phönix	Cloridrato de oxibutinina	18A12-B03-349624	1
Sanacorp	Cloridrato de oxibutinina	18A12-B03-353049	1

- 235 868 spectra from 1515 *Apo-Ident* customers from a total of 49 175 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de oxibutinina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de oxibutinina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	265	0	152 697
Type B	0	380	0	201 704
Type C	0	199	0	235 868

The substance/substance group *Cloridrato de oxibutinina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7358 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.9849 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21543	21543	0,00	176,31
21704	25457	4,44	174,32
22732	21543	5,03	177,35
25059	25351	9,50	178,42
25351	25351	0,00	179,68
25457	25457	0,00	175,67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de oxitetraciclina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20090-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de oxitetraciclina; Oxitetraciclina, cloridrato; Oxytetracyclini hydrochloridum

Special notes

When selecting the *Cloridrato de oxitetraciclina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de oxitetraciclina	13	4	150

Second-stage model

For differentiation of the substance/substance group *Cloridrato de oxitetraciclina* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de oxitetraciclina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	57,63	–
⋮	⋮	⋮
Cloreto de dequalínio	>50	49,57
Eosina amarela	>50	77,50
Tanino	>50	115,48
Levotiroxina sódica	>50	128,08
Ditranol	>50	227,76
Ácido acetilsalicílico	>50	393,73
Salicilato de sódio	>50	430,92
Ácido benzoico	>50	496,47

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de oxitetraciclina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de oxitetraciclina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de oxitetraciclina	12130001	20847	40	20120530
Caelo	Cloridrato de oxitetraciclina	12328103	21039	40	20121214
Caelo	Cloridrato de oxitetraciclina	16077002	22503	40	AR-16-FG-011460-01
Euro OTC	Cloridrato de oxitetraciclina	1306022-02	21600	60	1507542
Euro OTC	Cloridrato de oxitetraciclina	1506037	21836	60	20150721*
Euro OTC	Cloridrato de oxitetraciclina	1506037	21999	60	20150721*
Euro OTC	Cloridrato de oxitetraciclina	1602025	22546	40	20160609*
Euro OTC	Cloridrato de oxitetraciclina	1602025-01	22658	40	AR-16-FG-014422-01
Euro OTC	Cloridrato de oxitetraciclina	1602025	22669	40	20160609*
Euro OTC	Cloridrato de oxitetraciclina	1602025-02	22839	40	20161021
Euro OTC	Cloridrato de oxitetraciclina	1602025-02	22846	40	20161021
Euro OTC	Cloridrato de oxitetraciclina	1701034	23137	40	20170314*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cloridrato de oxitetraciclina	1701035-02	23970	40	20170314
Euro OTC	Cloridrato de oxitetraciclina	2103010	25657	40	20210420*
Fagron	Cloridrato de oxitetraciclina	13D08-N11	20848	60	20110131
Fagron	Cloridrato de oxitetraciclina	15D29-B99-309066	21915	60	20150522

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 740 spectra of 16 reference samples from the substance/substance group *Cloridrato de oxitetraciclina*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 222 spectra from a total of 2829 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Cloridrato de oxitetraciclina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de oxitetraciclina	173168	23786	40
Euro OTC	Cloridrato de oxitetraciclina	1801033	23971	40
Euro OTC	Cloridrato de oxitetraciclina	2310021	27275	40
Fagron	Cloridrato de oxitetraciclina	15L16-B02-322908	23226	40
Caelo	Cloridrato de oxitetraciclina	12130001	20847†	20
Euro OTC	Cloridrato de oxitetraciclina	2310021	27275SI	20
Fagron	Cloridrato de oxitetraciclina	15L16-B02-322908	23417	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1014 spectra from 431 *Apo-Ident* customers from 167 batches from the substance/substance group *Cloridrato de oxitetraciclina*.
- Among them are spectra of independent samples from 149 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de oxitetraciclina		1
	Cloridrato de oxitetraciclina	10305038	1
	Cloridrato de oxitetraciclina	130602202	1
	Cloridrato de oxitetraciclina	1306022-02	3
	Cloridrato de oxitetraciclina	140701201	1
	Cloridrato de oxitetraciclina	2103010-03	5
	Cloridrato de oxitetraciclina	2310021-01	2
049	Cloridrato de oxitetraciclina	1801033-01	1
AHD	Cloridrato de oxitetraciclina	1602025-01	1
AHD	Cloridrato de oxitetraciclina	17316805	1
AHD	Cloridrato de oxitetraciclina	17316815	1
AHD	Cloridrato de oxitetraciclina	1801033-02	1
AHD	Cloridrato de oxitetraciclina	2103010-01	1
AHD	Cloridrato de oxitetraciclina	21030-10-03	1
Alliance Healthcare	Cloridrato de oxitetraciclina	1205028-02	1
Alliance Healthcare	Cloridrato de oxitetraciclina	1205222-01	1
Alliance Healthcare	Cloridrato de oxitetraciclina	2103010-01	2
Alliance	Cloridrato de oxitetraciclina	1407012-03	1
Anzag	Cloridrato de oxitetraciclina	12328103	1
Anzag	Cloridrato de oxitetraciclina	1506037	1
Anzag	Cloridrato de oxitetraciclina	1506037-02	1
Apoident	Cloridrato de oxitetraciclina	1602025-01	1
apomix	Cloridrato de oxitetraciclina	1602025-02	1
apomix	Cloridrato de oxitetraciclina	16077014	1
Bombastus	Cloridrato de oxitetraciclina	13L19-B33-290732	1
Bombastus	Cloridrato de oxitetraciclina	17316812	1
Bombastus	Cloridrato de oxitetraciclina	17316815	1
Bombastus	Cloridrato de oxitetraciclina	180103301	1
Caelo	Cloridrato de oxitetraciclina	1/01034-02	1
Caelo	Cloridrato de oxitetraciclina	11336507	1
Caelo	Cloridrato de oxitetraciclina	11336510	3
Caelo	Cloridrato de oxitetraciclina	12091405	1
Caelo	Cloridrato de oxitetraciclina	12130001	1
Caelo	Cloridrato de oxitetraciclina	12328103	1
Caelo	Cloridrato de oxitetraciclina	12328104	1
Caelo	Cloridrato de oxitetraciclina	12328107	1
Caelo	Cloridrato de oxitetraciclina	12G10-N04	1
Caelo	Cloridrato de oxitetraciclina	1306022-01	2
Caelo	Cloridrato de oxitetraciclina	13L19-B33	1
Caelo	Cloridrato de oxitetraciclina	13L19-B33-290730	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de oxitetraciclina	1407012-01	1
Caelo	Cloridrato de oxitetraciclina	14128003	1
Caelo	Cloridrato de oxitetraciclina	14128004	1
Caelo	Cloridrato de oxitetraciclina	14I22-B01-301463	1
Caelo	Cloridrato de oxitetraciclina	15060108	1
Caelo	Cloridrato de oxitetraciclina	15060109	9
Caelo	Cloridrato de oxitetraciclina	1506037	1
Caelo	Cloridrato de oxitetraciclina	1506037-01	5
Caelo	Cloridrato de oxitetraciclina	150603702	1
Caelo	Cloridrato de oxitetraciclina	1506037-02	1
Caelo	Cloridrato de oxitetraciclina	1602025-01	1
Caelo	Cloridrato de oxitetraciclina	160202502	3
Caelo	Cloridrato de oxitetraciclina	1602025-02	4
Caelo	Cloridrato de oxitetraciclina	16044007	1
Caelo	Cloridrato de oxitetraciclina	16077001	3
Caelo	Cloridrato de oxitetraciclina	16077002	2
Caelo	Cloridrato de oxitetraciclina	16077003	3
Caelo	Cloridrato de oxitetraciclina	16077007	2
Caelo	Cloridrato de oxitetraciclina	16077008	7
Caelo	Cloridrato de oxitetraciclina	16077009	1
Caelo	Cloridrato de oxitetraciclina	16077011	2
Caelo	Cloridrato de oxitetraciclina	16077012	1
Caelo	Cloridrato de oxitetraciclina	16077015	1
Caelo	Cloridrato de oxitetraciclina	16077016	2
Caelo	Cloridrato de oxitetraciclina	16077017	1
Caelo	Cloridrato de oxitetraciclina	1607716	1
Caelo	Cloridrato de oxitetraciclina	163406010	1
Caelo	Cloridrato de oxitetraciclina	16340605	4
Caelo	Cloridrato de oxitetraciclina	16340606	3
Caelo	Cloridrato de oxitetraciclina	16340609	1
Caelo	Cloridrato de oxitetraciclina	16340610	15
Caelo	Cloridrato de oxitetraciclina	16340611	2
Caelo	Cloridrato de oxitetraciclina	16340616	1
Caelo	Cloridrato de oxitetraciclina	1701034-01	1
Caelo	Cloridrato de oxitetraciclina	1701034-02	9
Caelo	Cloridrato de oxitetraciclina	1716819	1
Caelo	Cloridrato de oxitetraciclina	17316805	6
Caelo	Cloridrato de oxitetraciclina	17316806	4
Caelo	Cloridrato de oxitetraciclina	17316809	1
Caelo	Cloridrato de oxitetraciclina	17316811	4
Caelo	Cloridrato de oxitetraciclina	17316812	3
Caelo	Cloridrato de oxitetraciclina	17316815	6
Caelo	Cloridrato de oxitetraciclina	17316816	1
Caelo	Cloridrato de oxitetraciclina	17316819	1
Caelo	Cloridrato de oxitetraciclina	17316820	2
Caelo	Cloridrato de oxitetraciclina	1801033-01	1
Caelo	Cloridrato de oxitetraciclina	21021305	1
Caelo	Cloridrato de oxitetraciclina	5041402	1
Caesar & Loretz GmbH...	Cloridrato de oxitetraciclina	17316815	2
Caesar & Loretz GmbH	Cloridrato de oxitetraciclina	17316815	1
Caesar & Loretz Hilden	Cloridrato de oxitetraciclina	17316815	1
Caesar u. Loretz/Noweda	Cloridrato de oxitetraciclina	1602025-02	1
Caesar&Loretz GmbH	Cloridrato de oxitetraciclina	15060109	1
Caesar&Loretz	Cloridrato de oxitetraciclina	16340610	1
caesar	Cloridrato de oxitetraciclina	16077008	2
Caleo/ Noweda	Cloridrato de oxitetraciclina	16340616	1
Caleo/ Noweda	Cloridrato de oxitetraciclina	17316805	1
Century Pharmaceutic...	Cloridrato de oxitetraciclina	10305038-OH	1
Century Pharmaceuticals	Cloridrato de oxitetraciclina	2103010-01	1
Ebert & Jacobi	Cloridrato de oxitetraciclina	1701034-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Eu Rho Pharm/G	Cloridrato de oxitetraciclina	2103010-01	1
EuRho / Gehe	Cloridrato de oxitetraciclina	2103010-03	1
EuRho/Alliance Healt...	Cloridrato de oxitetraciclina	1801033-01	1
EuRho/Alliance	Cloridrato de oxitetraciclina	1801033-01	1
EuRho/Gehe	Cloridrato de oxitetraciclina	1801033-02	1
EuRho/Phönix	Cloridrato de oxitetraciclina	YT170302019	1
EuRho	Cloridrato de oxitetraciclina	1111061-01	1
EuRho	Cloridrato de oxitetraciclina	1205028-01	2
EuRho	Cloridrato de oxitetraciclina	2103010-03	1
Euro OTC	Cloridrato de oxitetraciclina		2
Euro OTC	Cloridrato de oxitetraciclina	1011045-01	3
Euro OTC	Cloridrato de oxitetraciclina	10305038	1
Euro OTC	Cloridrato de oxitetraciclina	10305038-OH	3
Euro OTC	Cloridrato de oxitetraciclina	1111061-01	6
Euro OTC	Cloridrato de oxitetraciclina	1111061-61	1
Euro OTC	Cloridrato de oxitetraciclina	11701034-02	1
Euro OTC	Cloridrato de oxitetraciclina	1205028	1
Euro OTC	Cloridrato de oxitetraciclina	12050-28	1
Euro OTC	Cloridrato de oxitetraciclina	1205028-01	6
Euro OTC	Cloridrato de oxitetraciclina	120502802	2
Euro OTC	Cloridrato de oxitetraciclina	1205028-02	14
Euro OTC	Cloridrato de oxitetraciclina	1306022	1
Euro OTC	Cloridrato de oxitetraciclina	130602201	2
Euro OTC	Cloridrato de oxitetraciclina	1306022-01	24
Euro OTC	Cloridrato de oxitetraciclina	130602202	1
Euro OTC	Cloridrato de oxitetraciclina	1306022-02	14
Euro OTC	Cloridrato de oxitetraciclina	1306022-03	5
Euro OTC	Cloridrato de oxitetraciclina	1407011202	1
Euro OTC	Cloridrato de oxitetraciclina	1407012-01	17
Euro OTC	Cloridrato de oxitetraciclina	1407012-02	17
Euro OTC	Cloridrato de oxitetraciclina	140701203	1
Euro OTC	Cloridrato de oxitetraciclina	1407012-03	5
Euro OTC	Cloridrato de oxitetraciclina	1407012-09	1
Euro OTC	Cloridrato de oxitetraciclina	1407012-1	1
Euro OTC	Cloridrato de oxitetraciclina	15051507	1
Euro OTC	Cloridrato de oxitetraciclina	15060109	1
Euro OTC	Cloridrato de oxitetraciclina	1506037	3
Euro OTC	Cloridrato de oxitetraciclina	150603701	1
Euro OTC	Cloridrato de oxitetraciclina	1506037-01	31
Euro OTC	Cloridrato de oxitetraciclina	1506037-02	32
Euro OTC	Cloridrato de oxitetraciclina	1506037-03	19
Euro OTC	Cloridrato de oxitetraciclina	15060377-01	1
Euro OTC	Cloridrato de oxitetraciclina	16020228-02	1
Euro OTC	Cloridrato de oxitetraciclina	1602025	3
Euro OTC	Cloridrato de oxitetraciclina	1602025_01	1
Euro OTC	Cloridrato de oxitetraciclina	160202501	2
Euro OTC	Cloridrato de oxitetraciclina	1602025-01	23
Euro OTC	Cloridrato de oxitetraciclina	160202502	1
Euro OTC	Cloridrato de oxitetraciclina	1602025-02	55
Euro OTC	Cloridrato de oxitetraciclina	1602025-1	1
Euro OTC	Cloridrato de oxitetraciclina	162025-02	1
Euro OTC	Cloridrato de oxitetraciclina	170034-01	1
Euro OTC	Cloridrato de oxitetraciclina	17010301	1
Euro OTC	Cloridrato de oxitetraciclina	1701034	1
Euro OTC	Cloridrato de oxitetraciclina	170103401	2
Euro OTC	Cloridrato de oxitetraciclina	1701034-01	51
Euro OTC	Cloridrato de oxitetraciclina	1701034-0104915216	1
Euro OTC	Cloridrato de oxitetraciclina	1701034-015415	1
Euro OTC	Cloridrato de oxitetraciclina	170103402	3
Euro OTC	Cloridrato de oxitetraciclina	1701034-02	59

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de oxitetraciclina	170313OH/1602025-01	1
Euro OTC	Cloridrato de oxitetraciclina	170612181	1
Euro OTC	Cloridrato de oxitetraciclina	171034-02	1
Euro OTC	Cloridrato de oxitetraciclina	18010322-02	1
Euro OTC	Cloridrato de oxitetraciclina	1801033	6
Euro OTC	Cloridrato de oxitetraciclina	1801033_02	1
Euro OTC	Cloridrato de oxitetraciclina	180103301	5
Euro OTC	Cloridrato de oxitetraciclina	1801033-01	92
Euro OTC	Cloridrato de oxitetraciclina	1801033-01P-190311-2	1
Euro OTC	Cloridrato de oxitetraciclina	180103302	3
Euro OTC	Cloridrato de oxitetraciclina	1801033-02	56
Euro OTC	Cloridrato de oxitetraciclina	1801033-1	1
Euro OTC	Cloridrato de oxitetraciclina	1801033-22	1
Euro OTC	Cloridrato de oxitetraciclina	181016183	1
Euro OTC	Cloridrato de oxitetraciclina	2102010-03	1
Euro OTC	Cloridrato de oxitetraciclina	210301001	1
Euro OTC	Cloridrato de oxitetraciclina	2103010-01	49
Euro OTC	Cloridrato de oxitetraciclina	210301002	1
Euro OTC	Cloridrato de oxitetraciclina	2103010-02	11
Euro OTC	Cloridrato de oxitetraciclina	2103010-03	21
Euro OTC	Cloridrato de oxitetraciclina	21111815	1
Euro OTC	Cloridrato de oxitetraciclina	28011505	1
Euro OTC	Cloridrato de oxitetraciclina	375-18	1
Euro OTC	Cloridrato de oxitetraciclina	513E-02865	1
Euro OTC	Cloridrato de oxitetraciclina	YT150502056	1
Euro OTC	Cloridrato de oxitetraciclina	YT160702059	2
Euro OTC	Cloridrato de oxitetraciclina	YT170302019	1
Euro/ Jenne	Cloridrato de oxitetraciclina	1801033-01	1
Euro/Gehe	Cloridrato de oxitetraciclina	1602025-02	1
Euro/Gehe	Cloridrato de oxitetraciclina	170103	1
Euro/Gehe	Cloridrato de oxitetraciclina	1701034-01	1
Euro/Gehe	Cloridrato de oxitetraciclina	181033-02	1
Euro/Gehe	Cloridrato de oxitetraciclina	2103010-01	2
Eurp OTG/AllianceHea...	Cloridrato de oxitetraciclina	1801033-01	1
Fagro/Anzag	Cloridrato de oxitetraciclina	14I22-B01-301464	1
Fagron	Cloridrato de oxitetraciclina		1
Fagron	Cloridrato de oxitetraciclina	12A26-N05	3
Fagron	Cloridrato de oxitetraciclina	12G10-N04	7
Fagron	Cloridrato de oxitetraciclina	130602203	1
Fagron	Cloridrato de oxitetraciclina	13D08-N11	6
Fagron	Cloridrato de oxitetraciclina	13I26-N11	1
Fagron	Cloridrato de oxitetraciclina	13L19-B33	4
Fagron	Cloridrato de oxitetraciclina	13L19-B33-290730	3
Fagron	Cloridrato de oxitetraciclina	13L19-B33-290731	2
Fagron	Cloridrato de oxitetraciclina	14/22-B01-301464	1
Fagron	Cloridrato de oxitetraciclina	14/22-B01-301465	1
Fagron	Cloridrato de oxitetraciclina	1407012-01	1
Fagron	Cloridrato de oxitetraciclina	14I22-B01	1
Fagron	Cloridrato de oxitetraciclina	14I22-B01-301464	1
Fagron	Cloridrato de oxitetraciclina	14I22-B01-301465	1
Fagron	Cloridrato de oxitetraciclina	14I22-B01-301463	1
Fagron	Cloridrato de oxitetraciclina	15D29-B99-308608	1
Fagron	Cloridrato de oxitetraciclina	15D29-B99-309066	1
Fagron	Cloridrato de oxitetraciclina	15D29-B99-309067	1
Fagron	Cloridrato de oxitetraciclina	15l16-b02-322907	1
Fagron	Cloridrato de oxitetraciclina	15L16-B02-322907	1
Fagron	Cloridrato de oxitetraciclina	15L16-B02-322908	1
Fagron	Cloridrato de oxitetraciclina	1701034-02	1
Fagron	Cloridrato de oxitetraciclina	1801033-01	1
Fagron	Cloridrato de oxitetraciclina	4-49732A-2	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de oxitetraciclina	912A-02865	1
Fagron	Cloridrato de oxitetraciclina	C22H25CIN209	1
Fagropn	Cloridrato de oxitetraciclina	13L19-B33-290731	1
Fiebig	Cloridrato de oxitetraciclina	1801033-01	1
Finteler Apotheke	Cloridrato de oxitetraciclina	1602025-02	2
Gehe amax	Cloridrato de oxitetraciclina	1506037-02	3
Gehe amax	Cloridrato de oxitetraciclina	150603737-03	1
Gehe amax	Cloridrato de oxitetraciclina	1701034-02	1
Gehe amax	Cloridrato de oxitetraciclina	1801033-01	1
Gehe amax	Cloridrato de oxitetraciclina	4-48969A	1
Gehe	Cloridrato de oxitetraciclina	1205028-01	1
Gehe	Cloridrato de oxitetraciclina	12A26-N05	2
Gehe	Cloridrato de oxitetraciclina	12g10-n04	1
Gehe	Cloridrato de oxitetraciclina	1306022-02	1
Gehe	Cloridrato de oxitetraciclina	1407012-03	1
Gehe	Cloridrato de oxitetraciclina	1602025-02	3
GEHE	Cloridrato de oxitetraciclina	1602025-02	1
GEHE	Cloridrato de oxitetraciclina	1701034-01	1
Gehe	Cloridrato de oxitetraciclina	1701034-02	1
Gehe	Cloridrato de oxitetraciclina	17316805	1
Gehe	Cloridrato de oxitetraciclina	1801033-01	3
Gehe	Cloridrato de oxitetraciclina	1801033-02	1
Gehe	Cloridrato de oxitetraciclina	2103010-01	1
Gehe	Cloridrato de oxitetraciclina	2103010-03	1
Ichthyol-Gesellschaft	Cloridrato de oxitetraciclina	1801033-01	2
L12	Cloridrato de oxitetraciclina	12328107	1
L12	Cloridrato de oxitetraciclina	16340610	1
L30	Cloridrato de oxitetraciclina	1701034-02	1
Laborchemie Apolda/Phönix	Cloridrato de oxitetraciclina	1506037-02	1
Nachprüfung vom 23.07.	Cloridrato de oxitetraciclina	91618269	1
Norbrook Lab.Ltd.	Cloridrato de oxitetraciclina	1506037-01	2
Norbrook/Gehe	Cloridrato de oxitetraciclina	140701203	1
Noweda/Euro	Cloridrato de oxitetraciclina	2103010-01	1
Noweda	Cloridrato de oxitetraciclina	140701202	1
Noweda	Cloridrato de oxitetraciclina	140701203	1
Noweda	Cloridrato de oxitetraciclina	1701034-01	1
Noweda	Cloridrato de oxitetraciclina	1701034-02	1
Noweda	Cloridrato de oxitetraciclina	1801033-01	2
noweda	Cloridrato de oxitetraciclina	2103010	1
Noweda	Cloridrato de oxitetraciclina	2103010-01	1
Noweda	Cloridrato de oxitetraciclina	2103010-03	3
Phoenix	Cloridrato de oxitetraciclina	1602025-02	1
Phoenix	Cloridrato de oxitetraciclina	17316817	1
Phoenix	Cloridrato de oxitetraciclina	3036	1
Phönix Gotha	Cloridrato de oxitetraciclina	1232814	1
Phönix Gotha	Cloridrato de oxitetraciclina	1407012-02	1
Phönix	Cloridrato de oxitetraciclina	1205028-01	1
Phönix	Cloridrato de oxitetraciclina	1701034-02	1
Puren Pharma GmbH / ...	Cloridrato de oxitetraciclina	17316816	1
Sanacorp Stralsund	Cloridrato de oxitetraciclina	2103010-02	1
Sanacorp	Cloridrato de oxitetraciclina	1701034-01	1
SANACORP	Cloridrato de oxitetraciclina	1801033-02	1
Yangzhou Liberty Pha...	Cloridrato de oxitetraciclina	1801033-01	1
Yangzhou Liberty Pharma	Cloridrato de oxitetraciclina	1801033-02	2

- 235 053 spectra from 1515 *Apo-Ident* customers from a total of 49 095 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de oxitetraciclina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de oxitetraciclina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	740	0	152 222
Type B	0	240	0	201 844
Type C	0	976	38	235 053

The substance/substance group *Cloridrato de oxitetraciclina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1892 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	96.2525 % (> 95.9566 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20847	21999	29,19	120,45
20848	21836	26,65	103,19
21039	21600	15,41	187,15
21600	21600	0,00	187,80
21836	21836	0,00	109,06
21915	21836	63,44	103,72
21999	21999	0,00	140,93
22503	22503	0,00	138,66
22546	22546	0,00	131,77
22658	22658	0,00	129,33
22669	22669	0,00	131,96
22839	22669	36,39	133,97
22846	22669	15,20	131,61

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23137	23137	0,00	146,58
23970	23137	37,98	146,47
25657	25657	0,00	169,72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de papaverina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20481-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de papaverina; Papaverina, cloridrato; Papaverini hydrochloridum

Special notes

When selecting the *Cloridrato de papaverina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de papaverina	5	3	15

Second-stage model

For differentiation of the substance/substance group *Cloridrato de papaverina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de papaverina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hemissuccinato de doxilamina	87,21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de papaverina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de papaverina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de papaverina	13324310	21735	60	20130920
Caelo	Cloridrato de papaverina	123161	23054	40	20121127*
Caelo	Cloridrato de papaverina	180876	25614	40	20180328*
Caelo	Cloridrato de papaverina	22003603	26502	30	20221216*
Caelo	Cloridrato de papaverina	22003603	26502SI	20	20221216*
Gatt-Koller	Cloridrato de papaverina	21J01628	27096	30	20210907

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 220 spectra of 6 reference samples from the substance/substance group *Cloridrato de papaverina*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 742 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Cloridrato de papaverina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de papaverina	163159	23053	40
Caelo	Cloridrato de papaverina	16315911	23928	40
Caelo	Cloridrato de papaverina	23001264	26851	40
Caelo	Cloridrato de papaverina	23001264	26851SI	20
Gatt-Koller	Cloridrato de papaverina	21J01628	27096SI†	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 11 *Apo-Ident* customers from 16 batches from the substance/substance group *Cloridrato de papaverina*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de papaverina		1
Caelo	Cloridrato de papaverina	12166105	1
Caelo	Cloridrato de papaverina	12166112	1
Caelo	Cloridrato de papaverina	12316105	1
Caelo	Cloridrato de papaverina	13324307	1
Caelo	Cloridrato de papaverina	15160601	1
Caelo	Cloridrato de papaverina	15160608	2
Caelo	Cloridrato de papaverina	16315903	1
Caelo	Cloridrato de papaverina	16315907	1
Caelo	Cloridrato de papaverina	16315911	1
Caelo	Cloridrato de papaverina	17358802	1
Caelo	Cloridrato de papaverina	1817Q-02043	1
Fagron	Cloridrato de papaverina	21F07-B09	2
GATT-KOLLER/PHOENIX	Cloridrato de papaverina	2927/07131314	1
Phönix Gotha	Cloridrato de papaverina	12166101	1
Phönix Gotha	Cloridrato de papaverina	13324306	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de papaverina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de papaverina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	160	0	201 924
Type C	0	17	1	236 049

The substance/substance group *Cloridrato de papaverina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21735	26502	18,29	138,12
23054	23054	0,00	138,59
25614	25614	0,00	137,58
26502	26502	0,00	137,35
27096	23054	8,34	139,99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de pilocarpina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21519-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de pilocarpina; Pilocarpina, cloridrato; Pilocarpini hydrochloridum

Special notes

When selecting the *Cloridrato de pilocarpina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de pilocarpina	7	6	56

Second-stage model

For differentiation of the substance/substance group *Cloridrato de pilocarpina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de pilocarpina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ofloxacino	52,17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de pilocarpina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de pilocarpina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de pilocarpina	12217319	21518	60	20120806
Caelo	Cloridrato de pilocarpina	12217319	21519	60	1501660
Caelo	Cloridrato de pilocarpina	171595	23337	40	20170606*
Caelo	Cloridrato de pilocarpina	17124208	23371	40	20170607
Euro OTC	Cloridrato de pilocarpina	1305044-01	21629	60	20130725
Euro OTC	Cloridrato de pilocarpina	1305044-01	21629SI	60	20130725
Euro OTC	Cloridrato de pilocarpina	1603047	22553	40	20160429*
Euro OTC	Cloridrato de pilocarpina	1603047	22553SI	40	20160429*
Euro OTC	Cloridrato de pilocarpina	1908008	24845	40	20190830*
Fagron	Cloridrato de pilocarpina	22H16-B10-221817	26386	40	20220912
Fagron	Cloridrato de pilocarpina	22H16-B10-221817	26386SI	40	20220912

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 520 spectra of 11 reference samples from the substance/substance group *Cloridrato de pilocarpina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 442 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 660 spectra of 16 reference samples from the substance/substance group *Cloridrato de pilocarpina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de pilocarpina	171242	23338	40
Caelo	Cloridrato de pilocarpina	191220	24762	40
Caelo	Cloridrato de pilocarpina	23000207	26727	40
Euro OTC	Cloridrato de pilocarpina	1806012	24140	40
Euro OTC	Cloridrato de pilocarpina	2010012	25478	40
Euro OTC	Cloridrato de pilocarpina	2208009	26270	40
Caelo	Cloridrato de pilocarpina	12217319	21518SI†	60
Caelo	Cloridrato de pilocarpina	171595	23337SI†	40
Caelo	Cloridrato de pilocarpina	171242	23338SI	40
Caelo	Cloridrato de pilocarpina	17124208	23371SI†	40
Caelo	Cloridrato de pilocarpina	191220	24762SI	40
Caelo	Cloridrato de pilocarpina	23000207	26727SI	40
Euro OTC	Cloridrato de pilocarpina	1806012	24140SI	40
Euro OTC	Cloridrato de pilocarpina	1908008	24845SI†	40
Euro OTC	Cloridrato de pilocarpina	2010012	25478SI	40
Euro OTC	Cloridrato de pilocarpina	2208009	26270SI	40

- 201 424 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 189 spectra from 107 *Apo-Ident* customers from 60 batches from the substance/substance group *Cloridrato de pilocarpina*.
- Among them are spectra of independent samples from 56 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de pilocarpina	2208009-01	2
	Cloridrato de pilocarpina	23000207002	1
	Cloridrato de pilocarpina	24001858003	1
1806012-01	Cloridrato de pilocarpina	15198603	1
1Caesar & Loretz GmbH	Cloridrato de pilocarpina	21001750010	1
Caelo	Cloridrato de pilocarpina	11161903	1
Caelo	Cloridrato de pilocarpina	12217302	1
Caelo	Cloridrato de pilocarpina	12217307	1
Caelo	Cloridrato de pilocarpina	12217316	1
Caelo	Cloridrato de pilocarpina	12K07-N09	1
Caelo	Cloridrato de pilocarpina	130504401	1
Caelo	Cloridrato de pilocarpina	1305044-03	1
Caelo	Cloridrato de pilocarpina	14239402	1
Caelo	Cloridrato de pilocarpina	15198610	2
Caelo	Cloridrato de pilocarpina	15198701	2
Caelo	Cloridrato de pilocarpina	1603047-02	3
Caelo	Cloridrato de pilocarpina	17124208	4
Caelo	Cloridrato de pilocarpina	17159510	1
Caelo	Cloridrato de pilocarpina	17236401	1
Caelo	Cloridrato de pilocarpina	17332002	4
Caelo	Cloridrato de pilocarpina	18138704	6
Caelo	Cloridrato de pilocarpina	18138709	1
Caelo	Cloridrato de pilocarpina	191220001	5
Caelo	Cloridrato de pilocarpina	19122001	1
Caelo	Cloridrato de pilocarpina	21000139001	2
Caelo	Cloridrato de pilocarpina	21001750003	4
Caelo	Cloridrato de pilocarpina	2211112032607	1
Caelo	Cloridrato de pilocarpina	25051303	1
Caesar & Loretz GmbH...	Cloridrato de pilocarpina	191220001	1
Caesar & Loretz GmbH...	Cloridrato de pilocarpina	191220001	1
Caesar & Loretz GmbH...	Cloridrato de pilocarpina	191220009	4
Caesar & Loretz GmbH...	Cloridrato de pilocarpina	191220001	1
Caesar & Loretz GmbH	Cloridrato de pilocarpina	191220001	1
Caesar & Loretz GmbH	Cloridrato de pilocarpina	191220003	1
Caesar & Loretz GmbH	Cloridrato de pilocarpina	19122001	1
Caesar & Loretz GmbH	Cloridrato de pilocarpina	21000139001	1
Caesar & Loretz GmbH	Cloridrato de pilocarpina	21000139002	3
Caesar & Loretz GmbH	Cloridrato de pilocarpina	21000139005	4
Caesar & Loretz GmbH	Cloridrato de pilocarpina	21001750003	4
EuRho/Noweda	Cloridrato de pilocarpina	18060012-01	1
Euro OTC	Cloridrato de pilocarpina	1202031-01	1
Euro OTC	Cloridrato de pilocarpina	1202031-02	1
Euro OTC	Cloridrato de pilocarpina	13050-14-01	1
Euro OTC	Cloridrato de pilocarpina	130504401	2
Euro OTC	Cloridrato de pilocarpina	1305044-01	6
Euro OTC	Cloridrato de pilocarpina	1305044-03	2
Euro OTC	Cloridrato de pilocarpina	1603047	1
Euro OTC	Cloridrato de pilocarpina	1603047-01	6
Euro OTC	Cloridrato de pilocarpina	160304702	1
Euro OTC	Cloridrato de pilocarpina	1603047-02	28

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de pilocarpina	1806012-01	12
Euro OTC	Cloridrato de pilocarpina	1806012-02	4
Euro OTC	Cloridrato de pilocarpina	18CB02	1
Euro OTC	Cloridrato de pilocarpina	19008008-01	1
Euro OTC	Cloridrato de pilocarpina	190800	1
Euro OTC	Cloridrato de pilocarpina	1908008-01	16
Euro OTC	Cloridrato de pilocarpina	19CC02	1
Euro OTC	Cloridrato de pilocarpina	2010012-01	4
Euro OTC	Cloridrato de pilocarpina	Euroo	1
Euro OTG	Cloridrato de pilocarpina	1305044-01	1
Fagron	Cloridrato de pilocarpina	13H24-N03	1
Fagron	Cloridrato de pilocarpina	15B27-B03-309493	1
Fagron	Cloridrato de pilocarpina	18A31-B05-346072	1
Fagron	Cloridrato de pilocarpina	18A31-B05350799	1
Fagron	Cloridrato de pilocarpina	18A31-B05-350799	6
Fagron	Cloridrato de pilocarpina	19E20-B13-191235	1
Fagron	Cloridrato de pilocarpina	20D14-B05-196754	2
Fagron	Cloridrato de pilocarpina	20H18-B06-203134	1
Fagron	Cloridrato de pilocarpina	350799	1
Gehe	Cloridrato de pilocarpina	15198610	1
Gehe	Cloridrato de pilocarpina	17124209	1
Gehe	Cloridrato de pilocarpina	1806012-02	1
GEHE	Cloridrato de pilocarpina	18138704	1
Leyhs	Cloridrato de pilocarpina	15198701	1
Phönix	Cloridrato de pilocarpina	1603047-02	1
Sanacorp	Cloridrato de pilocarpina	12217302	1
SourcetechQuimica/Noweda	Cloridrato de pilocarpina		1

- 235 878 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de pilocarpina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de pilocarpina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	660	0	201 424
Type C	0	189	0	235 878

The substance/substance group *Cloridrato de pilocarpina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0909 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.8254 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21518	24845	23,47	57,54
21519	21519	0,00	62,23
21629	24845	6,40	61,55
22553	22553	0,00	65,55
23337	23337	0,00	67,49
23371	21519	7,15	61,48
24845	24845	0,00	61,91
26386	21519	30,59	73,32

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de piridoxina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20440-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de piridoxina; Piridoxina, cloridrato; Pyridoxini hydrochloridum

Special notes

When selecting the *Cloridrato de piridoxina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de piridoxina	8	12	60

Second-stage model

For differentiation of the substance/substance group *Cloridrato de piridoxina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de piridoxina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	119,58	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de piridoxina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de piridoxina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de piridoxina	14262302	21675	60	20141002
Caelo	Cloridrato de piridoxina	162225	22770	40	20160825*
Euro OTC	Cloridrato de piridoxina	1401044-01	21678	60	20140221
Euro OTC	Cloridrato de piridoxina	1407009-01	21773	60	20140807
Euro OTC	Cloridrato de piridoxina	1507012	21846	60	20150721*
Euro OTC	Cloridrato de piridoxina	1601039	22300	60	20160203*
Euro OTC	Cloridrato de piridoxina	2211006	26439	40	20221125*
Fagron	Cloridrato de piridoxina	22B07-B25-218396	26145	40	20220423

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 420 spectra of 8 reference samples from the substance/substance group *Cloridrato de piridoxina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 15 reference samples from the substance/substance group *Cloridrato de piridoxina*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de piridoxina	180287	24024	40
Caelo	Cloridrato de piridoxina	21004047002	25973	40
Caelo	Cloridrato de piridoxina	23001551	26839	40
Euro OTC	Cloridrato de piridoxina	1604063	22569	40
Euro OTC	Cloridrato de piridoxina	1608035	22798	40
Euro OTC	Cloridrato de piridoxina	1710014	23735	40
Euro OTC	Cloridrato de piridoxina	1806022-01	24189	40
Euro OTC	Cloridrato de piridoxina	1908009	24838	40
Euro OTC	Cloridrato de piridoxina	2107011	25778	50
Euro OTC	Cloridrato de piridoxina	2204009	26227	40
Euro OTC	Cloridrato de piridoxina	2309025	27001	40
Fagron	Cloridrato de piridoxina	24A17-B09-236138	27171	40
Caelo	Cloridrato de piridoxina	21004047002	25973SI	10
Euro OTC	Cloridrato de piridoxina	2204009	26227SI	20
Fagron	Cloridrato de piridoxina	22B07-B25-218396	26145SI†	20

- 201 544 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

provided by the customer regarding manufacturer and batch number.

- 125 spectra from 35 *Apo-Ident* customers from 61 batches from the substance/substance group *Cloridrato de piridoxina*.
- Among them are spectra of independent samples from 60 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de piridoxina	21004047010	1
	Cloridrato de piridoxina	24A17-B09-236138	1
Caelo	Cloridrato de piridoxina	11021406	1
Caelo	Cloridrato de piridoxina	11197009	1
Caelo	Cloridrato de piridoxina	12102510	1
Caelo	Cloridrato de piridoxina	12214102	2
Caelo	Cloridrato de piridoxina	12214119	2
Caelo	Cloridrato de piridoxina	13102509	2
Caelo	Cloridrato de piridoxina	13102510	2
Caelo	Cloridrato de piridoxina	13102516	1
Caelo	Cloridrato de piridoxina	14262302	3
Caelo	Cloridrato de piridoxina	14262306	1
Caelo	Cloridrato de piridoxina	15218702	6
Caelo	Cloridrato de piridoxina	15218707	1
Caelo	Cloridrato de piridoxina	15218709	1
Caelo	Cloridrato de piridoxina	15218710	2
Caelo	Cloridrato de piridoxina	15218713	3
Caelo	Cloridrato de piridoxina	16222501	5
Caelo	Cloridrato de piridoxina	16222504	1
Caelo	Cloridrato de piridoxina	16222506	2
Caelo	Cloridrato de piridoxina	16222514	3
Caelo	Cloridrato de piridoxina	16222515	2
Caelo	Cloridrato de piridoxina	16222520	1
Caelo	Cloridrato de piridoxina	16222521	1
Caelo	Cloridrato de piridoxina	18028703	2
Caelo	Cloridrato de piridoxina	18217603	1
Caelo	Cloridrato de piridoxina	18217614	1
Caelo	Cloridrato de piridoxina	19091203	2
Caelo	Cloridrato de piridoxina	20003108002	2
Caelo	Cloridrato de piridoxina	20003108003	1
Caelo	Cloridrato de piridoxina	21004047002	1
Caesar & Loretz GmbH...	Cloridrato de piridoxina	11197009	5
Caesar & Loretz GmbH...	Cloridrato de piridoxina	12214102	5
Caesar & Loretz GmbH...	Cloridrato de piridoxina	12214110	2
Caesar & Loretz GmbH...	Cloridrato de piridoxina	12214115	7
Caesar & Loretz GmbH...	Cloridrato de piridoxina	12214119	2
Caesar & Loretz GmbH...	Cloridrato de piridoxina	18217608	1
Caesar & Loretz GmbH...	Cloridrato de piridoxina	19091203	1
Caesar & Loretz GmbH	Cloridrato de piridoxina	18217603	1
Caesar & Loretz GmbH	Cloridrato de piridoxina	18217606	1
Caesar & Loretz GmbH	Cloridrato de piridoxina	18217608	5
Caesar & Loretz GmbH	Cloridrato de piridoxina	190912002	2
Caesar & Loretz GmbH	Cloridrato de piridoxina	19091203	1
Caesar & Loretz GmbH	Cloridrato de piridoxina	19091204	1
Caesar & Loretz GmbH	Cloridrato de piridoxina	21004047002	1
Euro OTC	Cloridrato de piridoxina	1110001-01	1
Euro OTC	Cloridrato de piridoxina	1206022-02	1
Euro OTC	Cloridrato de piridoxina	1601039-01	1
Euro OTC	Cloridrato de piridoxina	1604063-01	1
Euro OTC	Cloridrato de piridoxina	160803501	1
Euro OTC	Cloridrato de piridoxina	1608035-02	1
Euro OTC	Cloridrato de piridoxina	17001401	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de piridoxina	1710014-01	1
Euro OTC	Cloridrato de piridoxina	1806022-01	1
Euro OTC	Cloridrato de piridoxina	180602202	1
Euro OTC	Cloridrato de piridoxina	1908009-02	5
Euro OTC	Cloridrato de piridoxina	2204009-01	1
euro-oct	Cloridrato de piridoxina	UQ60313085/0	1
Fagron	Cloridrato de piridoxina	12e02-n02	1
Fagron	Cloridrato de piridoxina	1608035-01	1
Fagron	Cloridrato de piridoxina	20A29-F10-369782	1
Fagron	Cloridrato de piridoxina	21A25-F01-376555	2
Fagron	Cloridrato de piridoxina	21I01-B02-213683	1
Fagron	Cloridrato de piridoxina	L13080030	1
Farmalabor	Cloridrato de piridoxina	P1701531-000	1
Sanacorp	Cloridrato de piridoxina	21004047008	2
Sanacorp	Cloridrato de piridoxina	21004047010	2
Sanacorp	Cloridrato de piridoxina	2211006-02	1
Sanacorp	Cloridrato de piridoxina	23000263002	1
Sanacorp	Cloridrato de piridoxina	23000263003	3

- 235 942 spectra from 1515 *Apo-Ident* customers from a total of 49 197 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de piridoxina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de piridoxina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	540	0	201 544
Type C	0	125	0	235 942

The substance/substance group *Cloridrato de piridoxina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.2000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21675	21846	8,56	209,73
21678	21846	8,90	209,24
21773	21846	1,81	212,58
21846	21846	0,00	212,13
22300	22300	0,00	212,76
22770	22770	0,00	212,25
26145	21846	11,19	212,01
26439	26439	0,00	210,78

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de prilocaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21048-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de prilocaína; Prilocaína, cloridrato; Prilocaini hydrochloridum

Special notes

When selecting the *Cloridrato de prilocaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de prilocaína	4	3	20

Second-stage model

For differentiation of the substance/substance group *Cloridrato de prilocaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de prilocaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de anfetamina	79,14	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de prilocaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de prilocaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de prilocaína	15230305	21926	60	20150723
Fagron	Cloridrato de prilocaína	13I02-N03	21048	40	1403257
Fagron	Cloridrato de prilocaína	13I02-N03	21050	40	20130918
Fagron	Cloridrato de prilocaína	14H13-B03-297591	21800	60	AR-15-FG-016323-01
Fagron	Cloridrato de prilocaína	23A13-B01-225390	26612	40	20230208

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Cloridrato de prilocaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 722 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Cloridrato de prilocaína*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de prilocaína	15390101	23250	40
Fagron	Cloridrato de prilocaína	20B25-F04-369313	25484	40
Fagron	Cloridrato de prilocaína	24A16-B11-234645	27187	40
Fagron	Cloridrato de prilocaína	23A13-B01-225390	26612SI†	20
Fagron	Cloridrato de prilocaína	24A16-B11-234645	27187SI	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 35 spectra from 22 *Apo-Ident* customers from 23 batches from the substance/substance group *Cloridrato de prilocaína*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de prilocaína	21G10-B21-213674	3
Caelo	Cloridrato de prilocaína	14A03-B34-290281	1
Caelo	Cloridrato de prilocaína	15230304	1
Caelo	Cloridrato de prilocaína	15230305	1
Caelo	Cloridrato de prilocaína	15390101	1
Fagron	Cloridrato de prilocaína		1
Fagron	Cloridrato de prilocaína	13I032-N03	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de prilocaína	14H13-B03-297591	1
Fagron	Cloridrato de prilocaína	14H13-B03-297593	1
Fagron	Cloridrato de prilocaína	15E15-B04-307730	1
Fagron	Cloridrato de prilocaína	15L21-B02_332956	1
Fagron	Cloridrato de prilocaína	15L21-B02-319234	1
Fagron	Cloridrato de prilocaína	15L21-B02325756	1
Fagron	Cloridrato de prilocaína	15L21-B02332956	1
Fagron	Cloridrato de prilocaína	15L21-B02-332956	2
Fagron	Cloridrato de prilocaína	17H02-B05-340539	3
Fagron	Cloridrato de prilocaína	17H02-B05-348769	5
Fagron	Cloridrato de prilocaína	17Ho2Bo5348769	1
Fagron	Cloridrato de prilocaína	18B22-B04-356468	1
Fagron	Cloridrato de prilocaína	21F07-B14	1
Fagron	Cloridrato de prilocaína	21G10-B21-213674	1
Fagron	Cloridrato de prilocaína	F04-3766906	3
Fargon	Cloridrato de prilocaína	17H02-B05	1
GEHE 02.05.2013	Cloridrato de prilocaína		1

- 236 032 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de prilocaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de prilocaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	160	0	201 924
Type C	0	35	0	236 032

The substance/substance group *Cloridrato de prilocaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 82.8571 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21048	21048	0,00	101,52
21050	21048	3,52	102,24
21800	21800	0,00	104,65
21926	21800	4,59	101,43
26612	21048	11,17	104,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de procaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20042-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de procaína; Procaína, cloridrato; Procaini hydrochloridum

Special notes

When selecting the *Cloridrato de procaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de procaína	8	7	88

Second-stage model

For differentiation of the substance/substance group *Cloridrato de procaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de procaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	148,91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de procaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de procaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de procaína	13109906	21785	60	AR-15-FG-008935-01
Caelo	Cloridrato de procaína	15006906	22247	60	20150209
Caelo	Cloridrato de procaína	19000709003	25436	40	20200120
Caelo	Cloridrato de procaína	23000279004	26742	40	20230306
Caelo	Cloridrato de procaína	23000279004	26742SI	20	20230306
Euro OTC	Cloridrato de procaína	1601014	22306	60	20160203*
Euro OTC	Cloridrato de procaína	2210004	26442	40	20221116*
Fagron	Cloridrato de procaína	13F12-B40-301798	22260	60	20141210
Fagron	Cloridrato de procaína	15J27-B10-322937	23379	40	20151113

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 9 reference samples from the substance/substance group *Cloridrato de procaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 9 reference samples from the substance/substance group *Cloridrato de procaína*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de procaína	161378	22624	40
Caelo	Cloridrato de procaína	171675	23634	40
Caelo	Cloridrato de procaína	182764	24393	40
Caelo	Cloridrato de procaína	190440	24526	40
Caelo	Cloridrato de procaína	21003774005	26307	40
Caelo	Cloridrato de procaína	24001422	27309	30
Fagron	Cloridrato de procaína	22K02-B01-226161	26552	40
Caelo	Cloridrato de procaína	21003774005	26307SI	20
Fagron	Cloridrato de procaína	22K02-B01-226161	26552SI	20

- 201 774 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 208 spectra from 133 *Apo-Ident* customers from 92 batches from the substance/substance group *Cloridrato de procaína*.

- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de procaína	21003774005	1
	Cloridrato de procaína	22002755005	1
	Cloridrato de procaína	23000279003	1
	Cloridrato de procaína	23000279004	2
	Cloridrato de procaína	23000279007	1
	Cloridrato de procaína	23000279008	1
	Cloridrato de procaína	3000279004	1
Alliance Health 09.0...	Cloridrato de procaína	1104012-05	1
Anzag	Cloridrato de procaína	60998058	1
Caelo	Cloridrato de procaína	10159721	1
Caelo	Cloridrato de procaína	10159723	1
Caelo	Cloridrato de procaína	10159729	1
Caelo	Cloridrato de procaína	11370203	1
Caelo	Cloridrato de procaína	11370204	1
Caelo	Cloridrato de procaína	11370206	1
Caelo	Cloridrato de procaína	11370215	1
Caelo	Cloridrato de procaína	11370216	2
Caelo	Cloridrato de procaína	11370219	1
Caelo	Cloridrato de procaína	12177801	5
Caelo	Cloridrato de procaína	13/09-N08	1
Caelo	Cloridrato de procaína	13109905	1
Caelo	Cloridrato de procaína	13109906	1
Caelo	Cloridrato de procaína	13109908	2
Caelo	Cloridrato de procaína	13109915	1
Caelo	Cloridrato de procaína	13109916	2
Caelo	Cloridrato de procaína	131099903	1
Caelo	Cloridrato de procaína	13130-N06	1
Caelo	Cloridrato de procaína	13F12-B40-302510	1
Caelo	Cloridrato de procaína	14164408	1
Caelo	Cloridrato de procaína	14164409	1
Caelo	Cloridrato de procaína	14164413	1
Caelo	Cloridrato de procaína	15006902	1
Caelo	Cloridrato de procaína	15006906	3
Caelo	Cloridrato de procaína	15006909	1
Caelo	Cloridrato de procaína	15006912	4
Caelo	Cloridrato de procaína	15006913	1
Caelo	Cloridrato de procaína	1601014-02	1
Caelo	Cloridrato de procaína	16137812	5
Caelo	Cloridrato de procaína	16173906	2
Caelo	Cloridrato de procaína	17167504	1
Caelo	Cloridrato de procaína	17167505	1
Caelo	Cloridrato de procaína	17167506	2
Caelo	Cloridrato de procaína	17343306	1
Caelo	Cloridrato de procaína	17343311	1
Caelo	Cloridrato de procaína	18041806	1
Caelo	Cloridrato de procaína	18276407	4
Caelo	Cloridrato de procaína	19000709001	1
Caelo	Cloridrato de procaína	19000709003	9
Caelo	Cloridrato de procaína	19044008	2
Caelo	Cloridrato de procaína	192848001	1
Caelo	Cloridrato de procaína	192848002	7
Caelo	Cloridrato de procaína	192848005	1
Caelo	Cloridrato de procaína	20001278003	3
Caelo	Cloridrato de procaína	20001278004	2
Caelo	Cloridrato de procaína	20001278005	1
Caelo	Cloridrato de procaína	20004565003	3
Caelo	Cloridrato de procaína	20004565004	1
Caelo	Cloridrato de procaína	21003774002	6
Caelo	Cloridrato de procaína	22002755005	1
Caelo	Cloridrato de procaína	60998127	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de procaína	7011506	1
Caesar & Loretz GmbH...	Cloridrato de procaína	23000279004	1
Caesar & Loretz GmbH	Cloridrato de procaína	14164413	1
Caesar & Loretz GmbH	Cloridrato de procaína	17343306	1
Caesar & Loretz GmbH	Cloridrato de procaína	18276407	1
Caesar & Loretz GmbH	Cloridrato de procaína	19000709003	1
Caesar & Loretz GmbH	Cloridrato de procaína	19044008	1
CAESAR & LORETZ GMBH	Cloridrato de procaína	192848001	2
Caesar & Loretz GmbH	Cloridrato de procaína	192848005	1
Caesar & Loretz GmbH	Cloridrato de procaína	20001278003	1
Caesar & Loretz GmbH	Cloridrato de procaína	20004565003	1
Caesar & Loretz GmbH	Cloridrato de procaína	21003774002	1
Caesar & Loretz GmbH	Cloridrato de procaína	21003774005	3
Caesar & Loretz GmbH	Cloridrato de procaína	21003775002	1
China Medica	Cloridrato de procaína	13109911	1
Chongging Southwest No.2	Cloridrato de procaína	20001278004	1
Euro OTC	Cloridrato de procaína	1003001-01	1
Euro OTC	Cloridrato de procaína	1003001-02	1
Euro OTC	Cloridrato de procaína	1104012-01	1
Euro OTC	Cloridrato de procaína	1104012-03	3
Euro OTC	Cloridrato de procaína	1104012-04	3
Euro OTC	Cloridrato de procaína	1104012-05	4
Euro OTC	Cloridrato de procaína	1104012-3	1
Euro OTC	Cloridrato de procaína	1405027-01	4
Euro OTC	Cloridrato de procaína	1405027-02	1
Euro OTC	Cloridrato de procaína	16001014-02	1
Euro OTC	Cloridrato de procaína	1601014-01	9
Euro OTC	Cloridrato de procaína	1601014-02	22
Euro OTC	Cloridrato de procaína	1601014-02	1
Euro OTC	Cloridrato de procaína	16014014-02	1
Euro OTC	Cloridrato de procaína	200644	1
Euro OTC	Cloridrato de procaína	5127	1
Fagron	Cloridrato de procaína	10H11-N25	1
Fagron	Cloridrato de procaína	12I10-N07	1
Fagron	Cloridrato de procaína	13/30-N06	1
Fagron	Cloridrato de procaína	13F12-B40	1
Fagron	Cloridrato de procaína	13I09-N08	1
Fagron	Cloridrato de procaína	15006906	1
Fagron	Cloridrato de procaína	1651212	1
Fagron	Cloridrato de procaína	193768	1
Fagron	Cloridrato de procaína	20A30-B15-197566	1
Gatt-Koller / Phoenix	Cloridrato de procaína	4428/10122714	2
Gehe	Cloridrato de procaína	19044008	1
Guzugzhou Tengyue Ch...	Cloridrato de procaína	20201033	2
Herstellung	Cloridrato de procaína	12177801	1
Koisser	Cloridrato de procaína	11370218	1
Nachprüfung	Cloridrato de procaína	2082019-5	1
Noweda	Cloridrato de procaína	1309N08	1
Noweda	Cloridrato de procaína	1601014-02	1
Noweda	Cloridrato de procaína	22002755005	1
Noweda	Cloridrato de procaína	23000279004	1
Phönix 08.01.2014	Cloridrato de procaína	1104012-03	1
Phönix Gotha	Cloridrato de procaína	190311	1
Sanacorp	Cloridrato de procaína	20004565003	1
siehe WE-Prüfprotokoll	Cloridrato de procaína	39/12	1
VEB Jenapharmn	Cloridrato de procaína	1011989	1

- 235 859 spectra from 1515 *Apo-Ident* customers from a total of 49 166 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de procaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de procaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	310	0	201 774
Type C	0	208	0	235 859

The substance/substance group *Cloridrato de procaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.1154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21785	21785	0,00	197,01
22247	22306	6,74	199,31
22260	21785	6,88	198,14
22306	22306	0,00	197,16
23379	22306	3,21	197,44
25436	26442	13,77	202,75
26442	26442	0,00	201,13
26742	26442	9,42	203,92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de propranolol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20954-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de propranolol; Propranolol, cloridrato; Propranololi hydrochloridum

Special notes

When selecting the *Cloridrato de propranolol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de propranolol	6	5	197

Second-stage model

For differentiation of the substance/substance group *Cloridrato de propranolol* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de propranolol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	114,73	–
⋮	⋮	⋮
Sulfato de atropina	>50	78,49
Furoato de mometasona	>50	113,47
Fenitoína	>50	120,34
Sacarina sódica	>50	162,11
Quinolina amarela	>50	225,86
Sorbato de potássio	>50	228,46
Citrato monobásico de magnésio, hid…	>50	250,79
Hidrocortisona	>50	331,06
Orotato de cálcio di-hidratado	>50	432,33
Escina, hidrossolúvel	>50	620,18

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de propranolol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de propranolol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de propranolol	12370712	21396	60	20130116
Caelo	Cloridrato de propranolol	12370712	21410	60	20130116
Caelo	Cloridrato de propranolol	15283302	22590	40	20150929
Fagron	Cloridrato de propranolol	13I13-N04	20954	40	1402307
Fagron	Cloridrato de propranolol	15F16-B02-312979	22591	40	20150630
Fagron	Cloridrato de propranolol	18D23-B09-363591	25174	40	20180525
Fagron	Cloridrato de propranolol	20G30-F01-373061	25483	40	20200828

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Cloridrato de propranolol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Cloridrato de propranolol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de propranolol	171722	23650	40
Caelo	Cloridrato de propranolol	173330	23836	40
Caelo	Cloridrato de propranolol	192472	24878	40
Caelo	Cloridrato de propranolol	23000119	26718	40
Fagron	Cloridrato de propranolol	23A11-B01-224499	26616	40
Caelo	Cloridrato de propranolol	23000119	26718SI	20
Fagron	Cloridrato de propranolol	23A11-B01-224499	26616SI	20

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1512 spectra from 572 *Apo-Ident* customers from 215 batches from the substance/substance group *Cloridrato de propranolol*.

- Among them are spectra of independent samples from 195 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de propranolol	21002211012	3
	Cloridrato de propranolol	21002211013	2
	Cloridrato de propranolol	21002211014	3
	Cloridrato de propranolol	21002211016	2
	Cloridrato de propranolol	2100221104	1
	Cloridrato de propranolol	2102211012	1
	Cloridrato de propranolol	21J13-F02-380307	2
	Cloridrato de propranolol	21L01-B01-220233	1
	Cloridrato de propranolol	21L01-B01-222417	6
	Cloridrato de propranolol	23000119001	4
	Cloridrato de propranolol	23000119002	17
	Cloridrato de propranolol	2300119002	1
	Cloridrato de propranolol	230019002	1
	Cloridrato de propranolol	23003559002	2
	Cloridrato de propranolol	23E05-B05-229475	10
	Cloridrato de propranolol	23E05-B05-231731	2
	Cloridrato de propranolol	23E05-B05-233780	1
	Cloridrato de propranolol	B01-2241007	1
	Cloridrato de propranolol	B05-2317301	2
	Cloridrato de propranolol	B05-2337800	1
	Cloridrato de propranolol	B05-2378000	1
	Cloridrato de propranolol	M220726	2
/O. Geilenkirchen	Cloridrato de propranolol	15422502	1
AHD	Cloridrato de propranolol	15422501	1
AHD	Cloridrato de propranolol	17172204	2
AHD	Cloridrato de propranolol	17333001	1
AHD	Cloridrato de propranolol	17333006	1
AHD	Cloridrato de propranolol	18179402	3
AHD	Cloridrato de propranolol	941895	1
Alliance health	Cloridrato de propranolol	13E15-B40-294297	1
allianz	Cloridrato de propranolol	15283302	1
apomix	Cloridrato de propranolol	15K11-B01-316401	1
Audor Pharma	Cloridrato de propranolol	15K11-B01	1
cae	Cloridrato de propranolol	20003220002	1
Caelo	Cloridrato de propranolol		1
Caelo	Cloridrato de propranolol	12370703	1
Caelo	Cloridrato de propranolol	12370709	1
Caelo	Cloridrato de propranolol	12370710	1
Caelo	Cloridrato de propranolol	12370712	1
Caelo	Cloridrato de propranolol	12a27-n04	1
Caelo	Cloridrato de propranolol	12D27-N14	1
Caelo	Cloridrato de propranolol	13/13-N04	3
Caelo	Cloridrato de propranolol	13379804	1
Caelo	Cloridrato de propranolol	13379806	1
Caelo	Cloridrato de propranolol	13379807	5
Caelo	Cloridrato de propranolol	13379809	3
Caelo	Cloridrato de propranolol	13E15-B40-289355	2
Caelo	Cloridrato de propranolol	13I13N04	1
Caelo	Cloridrato de propranolol	150082405	1
Caelo	Cloridrato de propranolol	15082401	4
Caelo	Cloridrato de propranolol	15082404	1
Caelo	Cloridrato de propranolol	15082405	2
Caelo	Cloridrato de propranolol	15179405	1
Caelo	Cloridrato de propranolol	15283301	13
Caelo	Cloridrato de propranolol	15283302	5
Caelo	Cloridrato de propranolol	154225	1
Caelo	Cloridrato de propranolol	15422501	13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de propranolol	15422502	14
Caelo	Cloridrato de propranolol	15422505	7
Caelo	Cloridrato de propranolol	15422505-3032017/2	1
Caelo	Cloridrato de propranolol	1542251	1
Caelo	Cloridrato de propranolol	15F16-B02	1
Caelo	Cloridrato de propranolol	15F16-B02-312979	3
Caelo	Cloridrato de propranolol	15k11-B01	1
Caelo	Cloridrato de propranolol	15K11-B01-316401	1
Caelo	Cloridrato de propranolol	16138302	10
Caelo	Cloridrato de propranolol	16138302-3417/2	1
Caelo	Cloridrato de propranolol	16138304	16
Caelo	Cloridrato de propranolol	16138306	8
Caelo	Cloridrato de propranolol	1616E-03609	1
Caelo	Cloridrato de propranolol	16E09-B09-326637	3
Caelo	Cloridrato de propranolol	16E09-B09-330547	5
Caelo	Cloridrato de propranolol	16E09-B09-333442	1
Caelo	Cloridrato de propranolol	17106PRRII	1
Caelo	Cloridrato de propranolol	1712203	1
Caelo	Cloridrato de propranolol	1712204	1
Caelo	Cloridrato de propranolol	1712205	1
Caelo	Cloridrato de propranolol	17172203	22
Caelo	Cloridrato de propranolol	17172203-20112017/1	1
Caelo	Cloridrato de propranolol	17172204	18
Caelo	Cloridrato de propranolol	17172205	8
Caelo	Cloridrato de propranolol	1733001	1
Caelo	Cloridrato de propranolol	17333001	34
Caelo	Cloridrato de propranolol	173330015654	1
Caelo	Cloridrato de propranolol	17333005	1
Caelo	Cloridrato de propranolol	17333006	13
Caelo	Cloridrato de propranolol	17333008	1
Caelo	Cloridrato de propranolol	1733301	2
Caelo	Cloridrato de propranolol	1733306	1
Caelo	Cloridrato de propranolol	17K22-B03-342731	1
Caelo	Cloridrato de propranolol	17K22-B03-344247	2
Caelo	Cloridrato de propranolol	17K22-B03-345013	4
Caelo	Cloridrato de propranolol	17K22-B03-347251	5
Caelo	Cloridrato de propranolol	18179402	67
Caelo	Cloridrato de propranolol	18179403	34
Caelo	Cloridrato de propranolol	18179405	49
Caelo	Cloridrato de propranolol	18179406	1
Caelo	Cloridrato de propranolol	181799402	1
Caelo	Cloridrato de propranolol	18D23-B09	1
Caelo	Cloridrato de propranolol	18D23-B09-351774	6
Caelo	Cloridrato de propranolol	18D23-B09-355583	6
Caelo	Cloridrato de propranolol	18D23-B09-359713	5
Caelo	Cloridrato de propranolol	19242008	1
Caelo	Cloridrato de propranolol	19247001	1
Caelo	Cloridrato de propranolol	1924720008	1
Caelo	Cloridrato de propranolol	192472001	42
Caelo	Cloridrato de propranolol	192472002	1
Caelo	Cloridrato de propranolol	192472003	41
Caelo	Cloridrato de propranolol	192472008	25
Caelo	Cloridrato de propranolol	19272001	1
Caelo	Cloridrato de propranolol	20003220002	24
Caelo	Cloridrato de propranolol	20003220003	1
Caelo	Cloridrato de propranolol	20003220004	21
Caelo	Cloridrato de propranolol	2000322002	4
Caelo	Cloridrato de propranolol	2000322004	3
Caelo	Cloridrato de propranolol	2003220002	1
Caelo	Cloridrato de propranolol	2003220004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de propranolol	210002211001	1
Caelo	Cloridrato de propranolol	21002211001	39
Caelo	Cloridrato de propranolol	21002211002	23
Caelo	Cloridrato de propranolol	21002211007	20
Caelo	Cloridrato de propranolol	21002211010	14
Caelo	Cloridrato de propranolol	21002211012	22
Caelo	Cloridrato de propranolol	21002211013	11
Caelo	Cloridrato de propranolol	21002211014	2
Caelo	Cloridrato de propranolol	21002211016	2
Caelo	Cloridrato de propranolol	2100221102	5
Caelo	Cloridrato de propranolol	2100221107	1
Caelo	Cloridrato de propranolol	210507-01	1
Caelo	Cloridrato de propranolol	21052PRRII	1
Caelo	Cloridrato de propranolol	21J13-F02-380307	1
Caelo	Cloridrato de propranolol	23000119002	1
Caelo	Cloridrato de propranolol	2771	1
Caelo	Cloridrato de propranolol	m130104	1
Caelo	Cloridrato de propranolol	M130104	1
Caelo	Cloridrato de propranolol	M141203	1
Caelo	Cloridrato de propranolol	M180207	1
Caeo/Noweda	Cloridrato de propranolol	15283302	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	15422502	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	18179405	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	21002211010	2
Caesar & Loretz GmbH...	Cloridrato de propranolol	18179405	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	192472003	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	20003220002	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	20003220004	2
Caesar & Loretz GmbH...	Cloridrato de propranolol	18179403	5
Caesar & Loretz GmbH...	Cloridrato de propranolol	192472008	1
Caesar & Loretz GmbH/Gehe	Cloridrato de propranolol	20003220002	2
Caesar & Loretz GmbH/Gehe	Cloridrato de propranolol	21002211001	2
Caesar & Loretz GmbH/Gehe	Cloridrato de propranolol	21002211010	2
Caesar & Loretz GmbH/Gehe	Cloridrato de propranolol	21002211012	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	20003220002	2
Caesar & Loretz GmbH/Kehr	Cloridrato de propranolol	18179402	1
Caesar & Loretz GmbH/Kehr	Cloridrato de propranolol	18179405	1
Caesar & Loretz GmbH/Kehr	Cloridrato de propranolol	192472001	1
Caesar & Loretz GmbH/Kehr	Cloridrato de propranolol	21002211013	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	18179402	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	18179403	1
Caesar & Loretz GmbH/Otto	Cloridrato de propranolol	192472001	1
Caesar & Loretz GmbH/Otto	Cloridrato de propranolol	192472008	1
Caesar & Loretz GmbH/P	Cloridrato de propranolol	192472001	2
Caesar & Loretz GmbH...	Cloridrato de propranolol	192472001	3
Caesar & Loretz GmbH...	Cloridrato de propranolol	192472001	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	192472003	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	192472008	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	21002211002	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	20003220002	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	20003220004	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	21002211001	1
Caesar & Loretz GmbH...	Cloridrato de propranolol	21002211012	1
Caesar & Loretz GmbH	Cloridrato de propranolol		1
Caesar & Loretz GmbH	Cloridrato de propranolol	18179402	7
Caesar & Loretz GmbH	Cloridrato de propranolol	18179403	10
Caesar & Loretz GmbH	Cloridrato de propranolol	18179405	17
Caesar & Loretz GmbH	Cloridrato de propranolol	19247001	1
Caesar & Loretz GmbH	Cloridrato de propranolol	192472001	9
Caesar & Loretz GmbH	Cloridrato de propranolol	192472003	11

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de propranolol	192472008	19
Caesar & Loretz GmbH	Cloridrato de propranolol	20003220002	12
Caesar & Loretz GmbH	Cloridrato de propranolol	20003220004	10
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211001	16
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211002	7
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211007	15
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211010	4
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211012	12
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211013	1
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211014	2
Caesar & Loretz GmbH	Cloridrato de propranolol	21002211016	1
Caesar & Loretz GmbH	Cloridrato de propranolol	M180207	3
Caesar u Loretz	Cloridrato de propranolol	13379807	1
Caesar&Loretz GmbH	Cloridrato de propranolol	18179405	1
Caleo	Cloridrato de propranolol	192472008	1
Calo/AHD	Cloridrato de propranolol	15082401	1
Caselo	Cloridrato de propranolol	18179405	1
Cealo, GEHE	Cloridrato de propranolol	20003220002	1
Changhzhou Yabang Ph...	Cloridrato de propranolol	20G30-F01-373061	1
Changzhou / Faron	Cloridrato de propranolol	M151204	1
Changzhou / Gehe	Cloridrato de propranolol	M140808	1
Changzhou Yabang Pha...	Cloridrato de propranolol	15F16-B02	1
Euro OTC	Cloridrato de propranolol	13379806	1
Euro OTC	Cloridrato de propranolol	13I13-N04	1
Euro OTC	Cloridrato de propranolol	15K11B01-320607	1
Euro OTC	Cloridrato de propranolol	15K11-B01-322717	1
Euro OTC	Cloridrato de propranolol	16138304	2
Fagron	Cloridrato de propranolol		2
Fagron	Cloridrato de propranolol	10L20N08	2
Fagron	Cloridrato de propranolol	11D01-N11	1
Fagron	Cloridrato de propranolol	11I19-N09	1
Fagron	Cloridrato de propranolol	11L01-N05	2
Fagron	Cloridrato de propranolol	12A27-N04	1
Fagron	Cloridrato de propranolol	12D27-N14	4
Fagron	Cloridrato de propranolol	12F29-N06	4
Fagron	Cloridrato de propranolol	12F29-NO6	1
Fagron	Cloridrato de propranolol	12K06N07	1
Fagron	Cloridrato de propranolol	12K06-N07	7
Fagron	Cloridrato de propranolol	13/13-N04	4
Fagron	Cloridrato de propranolol	1313-N04	2
Fagron	Cloridrato de propranolol	13E15_B40-297021	1
Fagron	Cloridrato de propranolol	13E15-B40	5
Fagron	Cloridrato de propranolol	13E15-B40-289355	12
Fagron	Cloridrato de propranolol	13E15-B40-294297	5
Fagron	Cloridrato de propranolol	13E15-B40-297021	6
Fagron	Cloridrato de propranolol	13I13-N04	9
Fagron	Cloridrato de propranolol	13J13-N04	3
Fagron	Cloridrato de propranolol	13l13-N04	1
Fagron	Cloridrato de propranolol	15F16-B02	1
Fagron	Cloridrato de propranolol	15F16B02312979	1
Fagron	Cloridrato de propranolol	15F16-B02-312979	4
Fagron	Cloridrato de propranolol	15K11_B01_322717	1
Fagron	Cloridrato de propranolol	15K11-B01	4
Fagron	Cloridrato de propranolol	15K11-B01_320607	1
Fagron	Cloridrato de propranolol	15K11-B01-16401	1
Fagron	Cloridrato de propranolol	15K11-B01-316401	12
Fagron	Cloridrato de propranolol	15K11-B01-320607	8
Fagron	Cloridrato de propranolol	15K11-B01-322717	4
Fagron	Cloridrato de propranolol	15K11-Bo1-316401	1
Fagron	Cloridrato de propranolol	16138302	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de propranolol	16E09-B09	3
Fagron	Cloridrato de propranolol	16E09-B09-326637	16
Fagron	Cloridrato de propranolol	16E09B09330547	1
Fagron	Cloridrato de propranolol	16E09-B09-330547	7
Fagron	Cloridrato de propranolol	16E09-B09333442	1
Fagron	Cloridrato de propranolol	16E09-B09-333442	14
Fagron	Cloridrato de propranolol	17333001	1
Fagron	Cloridrato de propranolol	17K22-B03	5
Fagron	Cloridrato de propranolol	17K22-B03_347251	1
Fagron	Cloridrato de propranolol	17K22-B03-30048	1
Fagron	Cloridrato de propranolol	17k22-B03-342731	2
Fagron	Cloridrato de propranolol	17K22-B03-342731	8
Fagron	Cloridrato de propranolol	17K22-B03-344247	4
Fagron	Cloridrato de propranolol	17K22-B03-345013	1
Fagron	Cloridrato de propranolol	17K-22-B03-345013	1
Fagron	Cloridrato de propranolol	17k22-b03-347251	1
Fagron	Cloridrato de propranolol	17K22-B03-347251	5
Fagron	Cloridrato de propranolol	17K22-b03-350048	1
Fagron	Cloridrato de propranolol	17K22-B03-350048	6
Fagron	Cloridrato de propranolol	18041807	1
Fagron	Cloridrato de propranolol	18D_23-B09-351774	1
Fagron	Cloridrato de propranolol	18D23-B0	1
Fagron	Cloridrato de propranolol	18D23-B09	18
Fagron	Cloridrato de propranolol	18d23b09351774	1
Fagron	Cloridrato de propranolol	18D23-B09-351774	14
Fagron	Cloridrato de propranolol	18D23-B09-3555583	1
Fagron	Cloridrato de propranolol	18D23-B09-355583	10
Fagron	Cloridrato de propranolol	18D23-B09-357778	3
Fagron	Cloridrato de propranolol	18D23-B09-359713	19
Fagron	Cloridrato de propranolol	18D23-B09-363591	8
Fagron	Cloridrato de propranolol	20250711-8	1
Fagron	Cloridrato de propranolol	20G30-F01	4
Fagron	Cloridrato de propranolol	20G30-F01-0001	1
Fagron	Cloridrato de propranolol	20G30-F01-37	1
Fagron	Cloridrato de propranolol	20G30-F01-373060	17
Fagron	Cloridrato de propranolol	20G30-F01-373060/M200409	1
Fagron	Cloridrato de propranolol	20G30-F01-373061	12
Fagron	Cloridrato de propranolol	21J13-F02-380307	15
Fagron	Cloridrato de propranolol	21J3-F02_380307	1
Fagron	Cloridrato de propranolol	21j3-f02-380307	1
Fagron	Cloridrato de propranolol	21L01-B01-220233	1
Fagron	Cloridrato de propranolol	21L01-B01-222417	3
Fagron	Cloridrato de propranolol	23E05-B05-229475	2
Fagron	Cloridrato de propranolol	28051508	1
Fagron	Cloridrato de propranolol	3050PRII	1
Fagron	Cloridrato de propranolol	3050PRRII	2
Fagron	Cloridrato de propranolol	31101201	1
Fagron	Cloridrato de propranolol	3112U-03609	1
Fagron	Cloridrato de propranolol	3913M-03609	1
Fagron	Cloridrato de propranolol	4(20G30-F01-373060)	1
Fagron	Cloridrato de propranolol	402310015	1
Fagron	Cloridrato de propranolol	4071401	1
Fagron	Cloridrato de propranolol	5101	1
Fagron	Cloridrato de propranolol	700556-0001	1
Fagron	Cloridrato de propranolol	8D23-B09-3577781	1
Fagron	Cloridrato de propranolol	9CMK6AA71374	1
Fagron	Cloridrato de propranolol	9L09-N06	1
Fagron	Cloridrato de propranolol	B09-3597103	1
Fagron	Cloridrato de propranolol	B09-3635901	2
Fagron	Cloridrato de propranolol	F01-3730600	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de propranolol	F01-3730601	3
Fagron	Cloridrato de propranolol	M130104	1
Fagron	Cloridrato de propranolol	M141203	1
Fagron	Cloridrato de propranolol	M151204	3
Fagron	Cloridrato de propranolol	M170602	4
Fagron	Cloridrato de propranolol	M180207	6
Fagron	Cloridrato de propranolol	M200409	4
Fagron	Cloridrato de propranolol	M210630	1
Fargon/Noweda	Cloridrato de propranolol	18D23-B09-355583	2
Fargon	Cloridrato de propranolol	12K06-N07	1
Fargon	Cloridrato de propranolol	18D23-B09	1
Fargon	Cloridrato de propranolol	18D23-B09-359713	1
Fargon	Cloridrato de propranolol	M140808	1
fragon/AHD	Cloridrato de propranolol	13/13-N04	1
Fragon/Anzag	Cloridrato de propranolol	18D23-B09-359713	1
Gehe Kassel 26.06.2015	Cloridrato de propranolol	15082401	1
Gehe	Cloridrato de propranolol		1
Gehe	Cloridrato de propranolol	16E09-B09	1
Gehe	Cloridrato de propranolol	17172203	1
Gehe	Cloridrato de propranolol	17172205	2
Gehe	Cloridrato de propranolol	18179403	1
GEHE	Cloridrato de propranolol	18179405	1
Gehe	Cloridrato de propranolol	18D23	1
Gehe	Cloridrato de propranolol	192472003	1
Gehe	Cloridrato de propranolol	20003220004	1
Gehe	Cloridrato de propranolol	23000119002	1
Gehe	Cloridrato de propranolol	23E-05-B05-233780	1
Gutenberg-Apotheke	Cloridrato de propranolol	13I13-N04	1
Hedinger, Kehr /07.03.19	Cloridrato de propranolol	18179402	3
Ichthyol-Gesellschaf...	Cloridrato de propranolol	16138302	1
InfectoPharm	Cloridrato de propranolol	J0512011	1
Inresa 22.09.15	Cloridrato de propranolol	3043PRRII	1
IPCA / Noweda	Cloridrato de propranolol	192472003	2
Jenne	Cloridrato de propranolol	17333001	1
JENNE	Cloridrato de propranolol	17333001	1
Jenne	Cloridrato de propranolol	21002211001	2
Jenne	Cloridrato de propranolol	21002211013	1
Kehr	Cloridrato de propranolol	21L01-B01-222417	1
Kehr	Cloridrato de propranolol	23E05-B05-233780	1
Kehr	Cloridrato de propranolol	M180207	1
kontrolle	Cloridrato de propranolol	kontrolleAP210113-01	1
L12	Cloridrato de propranolol	16E09-B09-326637	1
L12	Cloridrato de propranolol	17K22-B03-350048	1
L12	Cloridrato de propranolol	18D23-B09-355583	1
L30	Cloridrato de propranolol	15K11-B01-320607	1
Land IpCA Laboratories	Cloridrato de propranolol	15422502	1
Löwen City-Apotheke ...	Cloridrato de propranolol	4012013	1
Nachprüfung	Cloridrato de propranolol	2082019-1	1
Noweda	Cloridrato de propranolol		1
Noweda	Cloridrato de propranolol	15K11-B01-322717	1
Noweda	Cloridrato de propranolol	17K22-B03-344247	2
Noweda	Cloridrato de propranolol	18179402	2
Noweda	Cloridrato de propranolol	18179405	2
Noweda	Cloridrato de propranolol	18179405/2x	1
Noweda	Cloridrato de propranolol	192472001	1
Noweda	Cloridrato de propranolol	192472008	1
Noweda	Cloridrato de propranolol	20003220002	1
Noweda	Cloridrato de propranolol	20003220004	1
Noweda	Cloridrato de propranolol	2100221002	1
Noweda	Cloridrato de propranolol	21002211012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Cloridrato de propranolol	23000119002	4
Noweda	Cloridrato de propranolol	23E05-B05-229475	1
Phoenix/Fargron	Cloridrato de propranolol	15K11-B01-322717	2
Phoenix	Cloridrato de propranolol	16138304	1
Phoenix	Cloridrato de propranolol	17K22-B03-344247	1
Phoenix	Cloridrato de propranolol	18179402	1
Phoenix	Cloridrato de propranolol	18D23-B09-355583	1
Phoenix	Cloridrato de propranolol	192472003	1
Phönix/Fragon	Cloridrato de propranolol	18D23-B09-357778	1
Phönix/Fragon	Cloridrato de propranolol	20G30-F01-373060	1
Phönix	Cloridrato de propranolol	15k11-b01-322717	1
Phönix	Cloridrato de propranolol	15k11-B01-322717	1
phönix	Cloridrato de propranolol	16e09-b09	1
phönix	Cloridrato de propranolol	16e09b09326637	1
Phönix	Cloridrato de propranolol	16E09-B09-326637	1
Phönix	Cloridrato de propranolol	17172203	1
Phönix	Cloridrato de propranolol	18179402	1
Phönix	Cloridrato de propranolol	192472003	2
phönix	Cloridrato de propranolol	2/AKD3	1
PHÖNIX	Cloridrato de propranolol	21002211002	1
Sanacorp	Cloridrato de propranolol	12370712	1
Sanacorp	Cloridrato de propranolol	16138304	1
Sanacorp	Cloridrato de propranolol	18D23-B09-351774	1
Sanacorp	Cloridrato de propranolol	20G30-F01	1
Sanacorp	Cloridrato de propranolol	21002211001	1
Sanacorp	Cloridrato de propranolol	23000119002	1
Sanacorp	Cloridrato de propranolol	23E05-B05-229475	1
VDL	Cloridrato de propranolol	18D23-B09-359713	1
WE:Phönix 12.08.2016	Cloridrato de propranolol	15422502	1

- 234 555 spectra from 1515 *Apo-Ident* customers from a total of 49 043 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de propranolol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de propranolol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	240	0	201 844
Type C	0	1505	7	234 555

The substance/substance group *Cloridrato de propranolol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	99.5370 % (> 99.3386 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20954	20954	0,00	235,69
21396	20954	4,29	233,71
21410	20954	21,77	233,80
22590	20954	9,07	234,04
22591	20954	25,34	239,55
25174	20954	34,90	241,04
25483	20954	44,61	241,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de quinina di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20547-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de quinina di-hidratado; Chinini hydrochloridum dihydricum; Quinina, cloridrato di-hidratado

Special notes

When selecting the *Cloridrato de quinina di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de quinina di-hidratado	7	3	15

Second-stage model

For differentiation of the substance/substance group *Cloridrato de quinina di-hidratado* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de quinina di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	84,47	–
⋮	⋮	⋮
Capsaicina	>50	160,26
Cloridrato de ciprofloxacina	>50	164,22
Citrato de sódio	>50	167,15
Cloridrato de oxibutinina	>50	194,60
Levocarnitina	>50	289,61
Heparina sódica	>50	299,85
Piridoxal-5-fosfato	>50	311,98
Metoxisaleno	>50	362,34
Prednicarbato	>50	379,50
Acetato de ciproterona	>50	471,39
Tetracaína	>50	519,15
Triclosan	>50	596,22
Alfaestradiol	>50	663,84
Sacarose	>50	894,45
Acetato de noretisterona	>50	1017,89
Cloridrato de amitriptilina	>50	1120,69
Amifampridina	>50	1150,67
Valina	>50	1652,84

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de quinina di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de quinina di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de quinina di-...	15376201	22309	60	20151105
Caelo	Cloridrato de quinina di-...	16283302	23577	40	1802260

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de quinina di-…	20002720	25621	40	20201119*
Fagron	Cloridrato de quinina di-…	13G10-N07	21235	30	20130809
Fagron	Cloridrato de quinina di-…	13I30-B02-295630	21809	60	AR-15-FG-015410-01
Fagron	Cloridrato de quinina di-…	20B26-F03-370029	25491	40	20200501
Fagron	Cloridrato de quinina di-…	21E06-B02-213598	26332	40	20210615
Fagron	Cloridrato de quinina di-…	21E06-B02-213598	26332SI	20	20210615

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 330 spectra of 8 reference samples from the substance/substance group *Cloridrato de quinina di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 632 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Cloridrato de quinina di-hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de quinina di-…	180226	24022	40
Fagron	Cloridrato de quinina di-…	15A20-B03-319027	23573	40
Fagron	Cloridrato de quinina di-…	16K01-B05-340171	23920	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 20 *Apo-Ident* customers from 18 batches from the substance/substance group *Cloridrato de quinina di-hidratado*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de quinina di-...	12316604	1
Caelo	Cloridrato de quinina di-...	12316605	1
Caelo	Cloridrato de quinina di-...	12316611	2
Caelo	Cloridrato de quinina di-...	12316617	1
Caelo	Cloridrato de quinina di-...	13D24-N06	1
Caelo	Cloridrato de quinina di-...	15227701	1
Caelo	Cloridrato de quinina di-...	15376201	2
Caelo	Cloridrato de quinina di-...	153776201	1
Caelo	Cloridrato de quinina di-...	153796204	1
Caelo	Cloridrato de quinina di-...	16283302	1
Caelo	Cloridrato de quinina di-...	16283305	3
Caelo	Cloridrato de quinina di-...	180226002	1
Caelo	Cloridrato de quinina di-...	18022602	1
Caelo	Cloridrato de quinina di-...	18022604	1
Caelo	Cloridrato de quinina di-...	18022605	1
Caesar & Loretz GmbH	Cloridrato de quinina di-...	180226002	1
Caesar & Loretz GmbH	Cloridrato de quinina di-...	18022605	1
Fagron	Cloridrato de quinina di-...	10N129B	1
Fagron	Cloridrato de quinina di-...	13G10-N07	1
Gatt-Koller	Cloridrato de quinina di-...	3500/08103810	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de quinina di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de quinina di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	330	0	152 632
Type B	0	120	0	201 964
Type C	0	24	0	236 043

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Cloridrato de quinina di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1818 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 75.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21235	25621	16,92	188,97
21809	21809	0,00	147,34
22309	23577	6,02	161,99
23577	23577	0,00	164,17
25491	23577	10,02	178,61
25621	25621	0,00	184,54
26332	21809	10,02	155,23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de ropivacaína monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10002307-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de ropivacaína monoidratado; Ropivacaína, cloridrato monoidratado; Ropivacaini hydrochloridum monohydricum

Special notes

When selecting the *Cloridrato de ropivacaína monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de ropivacaína monoidratado	5	2	0

Second-stage model

For differentiation of the substance/substance group *Cloridrato de ropivacaína monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de ropivacaína monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	78,07	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de ropivacaína monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de ropivacaína monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de ropivacaína…	181569	24871	40	20180802*
Euro OTC	Cloridrato de ropivacaína…	1707006	23704	40	20171013*
Euro OTC	Cloridrato de ropivacaína…	1903027	24607	40	20190416*
Fagron	Cloridrato de ropivacaína…	20I17-F09-375251	25920	40	2204443
Fagron	Cloridrato de ropivacaína…	22D25-B06	26444	40	20220812*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Cloridrato de ropivacaína monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Cloridrato de ropivacaína monoidratado*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de ropivacaína…	191139	24872	40
Euro OTC	Cloridrato de ropivacaína…	2106016	25919	40
Euro OTC	Cloridrato de ropivacaína…	2106016	25919SI	10

- 201 994 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cloridrato de ropivacaína monoidratado*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de ropivacaína monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For

this purpose, all relevant spectra of the various substances were compared with *Cloridrato de ropivacaína monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	90	0	201 994
Type C	0	0	0	236 067

The substance/substance group *Cloridrato de ropivacaína monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23704	23704	0,00	185,52
24607	24607	0,00	181,65
24871	24871	0,00	177,25
25920	25920	0,00	169,94
26444	26444	0,00	178,38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de sotalol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22656-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de sotalol; Sotalol, cloridrato; Sotaloli hydrochloridum

Special notes

When selecting the *Cloridrato de sotalol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de sotalol	3	1	1

Second-stage model

For differentiation of the substance/substance group *Cloridrato de sotalol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de sotalol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	135,71	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de sotalol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de sotalol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de sotalol	20000112	25199	40	20200210*
Caelo	Cloridrato de sotalol	24002039	27442	40	20241121*
Caelo	Cloridrato de sotalol	24002039	27442SI	20	20241121*
Fagron	Cloridrato de sotalol	21E21-B04-218998	26324	40	20210702
Fagron	Cloridrato de sotalol	21E21-B04-218998	26324SI	20	20210702

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 5 reference samples from the substance/substance group *Cloridrato de sotalol*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 802 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Cloridrato de sotalol*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Cloridrato de sotalol	369-MC	22656	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Cloridrato de sotalol*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Kehr	Cloridrato de sotalol	21001470007	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de sotalol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de sotalol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	40	0	202 044
Type C	0	1	0	236 066

The substance/substance group *Cloridrato de sotalol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25199	25199	0,00	222,44
26324	27442	4,51	222,85
27442	27442	0,00	221,63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de tetracaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20037-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de tetracaína; Tetracaína, cloridrato; Tetracaini hydrochloridum

Special notes

When selecting the *Cloridrato de tetracaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de tetracaína	8	20	386

Second-stage model

For differentiation of the substance/substance group *Cloridrato de tetracaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de tetracaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	168,23	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de tetracaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de tetracaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de tetracaína	12019822	20924	40	20120228
Caelo	Cloridrato de tetracaína	15437108	23163	40	20160211
Euro OTC	Cloridrato de tetracaína	1506040	21845	60	20150713*
Euro OTC	Cloridrato de tetracaína	1512019	22285	45	20151228*
Euro OTC	Cloridrato de tetracaína	1612005	22912	40	20170112*
Euro OTC	Cloridrato de tetracaína	1807017	24141	40	20180730*
Fagron	Cloridrato de tetracaína	15K04-B03-322151	23162	40	20160112
Fagron	Cloridrato de tetracaína	16G28-B03-327368	23500	40	20160826

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 345 spectra of 8 reference samples from the substance/substance group *Cloridrato de tetracaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 617 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 910 spectra of 26 reference samples from the substance/substance group *Cloridrato de tetracaína*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de tetracaína	190119	24561	40
Caelo	Cloridrato de tetracaína	22001496	26239	40
Euro OTC	Cloridrato de tetracaína	1607031	22708	40
Euro OTC	Cloridrato de tetracaína	1706018	23558	40
Euro OTC	Cloridrato de tetracaína	1712012	23886	40
Euro OTC	Cloridrato de tetracaína	1310006	23910	40
Euro OTC	Cloridrato de tetracaína	1803001	24079	40
Euro OTC	Cloridrato de tetracaína	1812006	24448	40
Euro OTC	Cloridrato de tetracaína	1902015	24452	40
Euro OTC	Cloridrato de tetracaína	1907007	24783	40
Euro OTC	Cloridrato de tetracaína	1909024	24974	40
Euro OTC	Cloridrato de tetracaína	2001011	25105	40
Euro OTC	Cloridrato de tetracaína	2003053	25267	40
Euro OTC	Cloridrato de tetracaína	2010019	25470	40
Euro OTC	Cloridrato de tetracaína	2110008	25885	50
Euro OTC	Cloridrato de tetracaína	2207015	26267	40
Euro OTC	Cloridrato de tetracaína	2307022	26879	30
Euro OTC	Cloridrato de tetracaína	2405009	27347	40
Fagron	Cloridrato de tetracaína	22J19-B01-221586	26551	40
Fagron	Cloridrato de tetracaína	24H26-B01-002406	27384	40
Caelo	Cloridrato de tetracaína	22001496	26239SI	20
Euro OTC	Cloridrato de tetracaína	2110008	25885SI	10
Euro OTC	Cloridrato de tetracaína	2207015	26267SI	20
Euro OTC	Cloridrato de tetracaína	2405009	27347SI	20
Fagron	Cloridrato de tetracaína	22J19-B01-221586	26551SI	20
Fagron	Cloridrato de tetracaína	24H26-B01-002406	27384SI	20

- 201 174 spectra from a total of 4025 batches from further 842 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2088 spectra from 718 *Apo-Ident* customers from 395 batches from the substance/substance group *Cloridrato de tetracaína*.
- Among them are spectra of independent samples from 383 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de tetracaína	1902015-01	1
	Cloridrato de tetracaína	1909024-01	1
	Cloridrato de tetracaína	2110008-01	3
	Cloridrato de tetracaína	21120-B04-225868	1
	Cloridrato de tetracaína	22001496004	1
	Cloridrato de tetracaína	22001496010	2
	Cloridrato de tetracaína	22001496014	1
	Cloridrato de tetracaína	22001496015	2
	Cloridrato de tetracaína	2201496015	1
	Cloridrato de tetracaína	2207015-01	7
	Cloridrato de tetracaína	2207015-02	1
	Cloridrato de tetracaína	2207015-03	3
	Cloridrato de tetracaína	221630	1
	Cloridrato de tetracaína	2307022-01	4
	Cloridrato de tetracaína	2405009-01	1
AHD/EuRho	Cloridrato de tetracaína	1902015-01	1
AHD	Cloridrato de tetracaína	15437121	1
AHD	Cloridrato de tetracaína	15A12-B03-308857	1
AHD	Cloridrato de tetracaína	18060602	1
AHD	Cloridrato de tetracaína	18060614	1
AHD	Cloridrato de tetracaína	2307022-01	1
AHD	Cloridrato de tetracaína	2405009-01	1
Alliance Health 05.0...	Cloridrato de tetracaína	13H21-B02-286559	1
Alliance Health 22.0...	Cloridrato de tetracaína	6093549	1
Alliance Health 30.0...	Cloridrato de tetracaína	1303012-01	2
Alliance Health	Cloridrato de tetracaína	14C18-B03-293967	1
Alliance Healthcare	Cloridrato de tetracaína	12H24-N05	1
Alliance	Cloridrato de tetracaína	220715-02	1
Anzag	Cloridrato de tetracaína	1411019-01	1
Anzag	Cloridrato de tetracaína	14710369	1
Anzag	Cloridrato de tetracaína	17256705	1
apo-ident	Cloridrato de tetracaína	1706018-01	1
Apolda/Gehe	Cloridrato de tetracaína	1909024	1
BASF Fine Chemicals ...	Cloridrato de tetracaína	13155714	1
BASF Pharma S.A.	Cloridrato de tetracaína	1310006-01	1
BASF Pharma S.A.	Cloridrato de tetracaína	1409026-02	1
BASF Pharma	Cloridrato de tetracaína	1411019-01	1
BASF	Cloridrato de tetracaína	13K25-B04-290277	1
BASF	Cloridrato de tetracaína	14C18-B03-293967	1
Bomastus / Alliance ...	Cloridrato de tetracaína	16G28-B03-327368	2
Bombastus	Cloridrato de tetracaína	13H21-B02-286558	1
Bombastus	Cloridrato de tetracaína	1712012-01	2
Caelo	Cloridrato de tetracaína	10118210	2
Caelo	Cloridrato de tetracaína	10118211	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de tetracaína	10118225	4
Caelo	Cloridrato de tetracaína	1110010-01	1
Caelo	Cloridrato de tetracaína	1110010-02	2
Caelo	Cloridrato de tetracaína	1110010-07	1
Caelo	Cloridrato de tetracaína	12019802	5
Caelo	Cloridrato de tetracaína	12019810	5
Caelo	Cloridrato de tetracaína	12019812	3
Caelo	Cloridrato de tetracaína	12019815	1
Caelo	Cloridrato de tetracaína	12019816	11
Caelo	Cloridrato de tetracaína	12019820	1
Caelo	Cloridrato de tetracaína	12019822	6
Caelo	Cloridrato de tetracaína	1207001-01	1
Caelo	Cloridrato de tetracaína	1260917/15437119	1
Caelo	Cloridrato de tetracaína	12H24-N05	1
Caelo	Cloridrato de tetracaína	1303012-01	1
Caelo	Cloridrato de tetracaína	1310006-01	1
Caelo	Cloridrato de tetracaína	1310006-02	1
Caelo	Cloridrato de tetracaína	1313012-01	1
Caelo	Cloridrato de tetracaína	13155703	1
Caelo	Cloridrato de tetracaína	13155705	3
Caelo	Cloridrato de tetracaína	13155706	10
Caelo	Cloridrato de tetracaína	13155711	7
Caelo	Cloridrato de tetracaína	13155714	2
Caelo	Cloridrato de tetracaína	13155716	2
Caelo	Cloridrato de tetracaína	13155720	2
Caelo	Cloridrato de tetracaína	13155724	4
Caelo	Cloridrato de tetracaína	13155727	6
Caelo	Cloridrato de tetracaína	13K25-B04-290276	1
Caelo	Cloridrato de tetracaína	1405026-01	1
Caelo	Cloridrato de tetracaína	1409026-02	3
Caelo	Cloridrato de tetracaína	1411019-01	4
Caelo	Cloridrato de tetracaína	14c18-b03-293966	1
Caelo	Cloridrato de tetracaína	14C18-B03-300199	1
Caelo	Cloridrato de tetracaína	14C18-B03-300200	1
Caelo	Cloridrato de tetracaína	14G14-B08	1
Caelo	Cloridrato de tetracaína	14G14-B08-300198	1
Caelo	Cloridrato de tetracaína	15/16-B06-312783	1
Caelo	Cloridrato de tetracaína	150604001	1
Caelo	Cloridrato de tetracaína	1506040-01	2
Caelo	Cloridrato de tetracaína	150604002	1
Caelo	Cloridrato de tetracaína	15079501	2
Caelo	Cloridrato de tetracaína	15079507	1
Caelo	Cloridrato de tetracaína	1508040-01	1
Caelo	Cloridrato de tetracaína	1512019-01	3
Caelo	Cloridrato de tetracaína	1512019-02	1
Caelo	Cloridrato de tetracaína	15196102	5
Caelo	Cloridrato de tetracaína	15196103	6
Caelo	Cloridrato de tetracaína	15196104	2
Caelo	Cloridrato de tetracaína	15356902	2
Caelo	Cloridrato de tetracaína	1537109	1
Caelo	Cloridrato de tetracaína	15437102	1
Caelo	Cloridrato de tetracaína	15437104	14
Caelo	Cloridrato de tetracaína	15437106	3
Caelo	Cloridrato de tetracaína	15437107	2
Caelo	Cloridrato de tetracaína	15437108	4
Caelo	Cloridrato de tetracaína	15437109	12
Caelo	Cloridrato de tetracaína	15437114	12
Caelo	Cloridrato de tetracaína	15437117	6
Caelo	Cloridrato de tetracaína	15437118	2
Caelo	Cloridrato de tetracaína	15437119	18

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de tetracaína	15437120	2
Caelo	Cloridrato de tetracaína	15437121	10
Caelo	Cloridrato de tetracaína	15437122	3
Caelo	Cloridrato de tetracaína	15H24-B03-311450	1
Caelo	Cloridrato de tetracaína	15K04-B03-318368	2
Caelo	Cloridrato de tetracaína	15K04-B03-318369	1
Caelo	Cloridrato de tetracaína	15K04-B03-328163	1
Caelo	Cloridrato de tetracaína	1607031-01	8
Caelo	Cloridrato de tetracaína	161200501	1
Caelo	Cloridrato de tetracaína	1612005-01	3
Caelo	Cloridrato de tetracaína	16G25-B03-332099	1
Caelo	Cloridrato de tetracaína	16G28-B03-332099	2
Caelo	Cloridrato de tetracaína	170601801	1
Caelo	Cloridrato de tetracaína	1706018-01	1
Caelo	Cloridrato de tetracaína	17114181	1
Caelo	Cloridrato de tetracaína	171201201	1
Caelo	Cloridrato de tetracaína	1712012-01	3
Caelo	Cloridrato de tetracaína	17256703	6
Caelo	Cloridrato de tetracaína	17256704	5
Caelo	Cloridrato de tetracaína	17256705	9
Caelo	Cloridrato de tetracaína	17G03-B07	1
Caelo	Cloridrato de tetracaína	17G03-B07-338538	2
Caelo	Cloridrato de tetracaína	17G03-B07-345008	2
Caelo	Cloridrato de tetracaína	17G03-B07-346693	1
Caelo	Cloridrato de tetracaína	1803001-01	16
Caelo	Cloridrato de tetracaína	1805019-01	1
Caelo	Cloridrato de tetracaína	18060602	20
Caelo	Cloridrato de tetracaína	18060603	6
Caelo	Cloridrato de tetracaína	18060604	4
Caelo	Cloridrato de tetracaína	18060606	1
Caelo	Cloridrato de tetracaína	18060609	2
Caelo	Cloridrato de tetracaína	18060610	1
Caelo	Cloridrato de tetracaína	18060612	10
Caelo	Cloridrato de tetracaína	18060613	1
Caelo	Cloridrato de tetracaína	18060614	5
Caelo	Cloridrato de tetracaína	18060619	2
Caelo	Cloridrato de tetracaína	18060620	8
Caelo	Cloridrato de tetracaína	18060621	3
Caelo	Cloridrato de tetracaína	18120006-01	1
Caelo	Cloridrato de tetracaína	1812006-01	3
Caelo	Cloridrato de tetracaína	18J03-B05	2
Caelo	Cloridrato de tetracaína	18J03-B05-361978	2
Caelo	Cloridrato de tetracaína	1901190002	1
Caelo	Cloridrato de tetracaína	190119001	9
Caelo	Cloridrato de tetracaína	190119002	3
Caelo	Cloridrato de tetracaína	190119003	1
Caelo	Cloridrato de tetracaína	19011901	7
Caelo	Cloridrato de tetracaína	19011903	8
Caelo	Cloridrato de tetracaína	19011903P-190909-2	1
Caelo	Cloridrato de tetracaína	19011906	3
Caelo	Cloridrato de tetracaína	19011907	9
Caelo	Cloridrato de tetracaína	19011908	9
Caelo	Cloridrato de tetracaína	20000156001	5
Caelo	Cloridrato de tetracaína	20000156002	1
Caelo	Cloridrato de tetracaína	20000156003	5
Caelo	Cloridrato de tetracaína	20000156005	7
Caelo	Cloridrato de tetracaína	20000156006	4
Caelo	Cloridrato de tetracaína	20000156008	7
Caelo	Cloridrato de tetracaína	200004176002	1
Caelo	Cloridrato de tetracaína	2000156003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de tetracaína	2000156005	1
Caelo	Cloridrato de tetracaína	2000156008	1
Caelo	Cloridrato de tetracaína	20004176003	9
Caelo	Cloridrato de tetracaína	20004176004	8
Caelo	Cloridrato de tetracaína	20004176006	4
Caelo	Cloridrato de tetracaína	20004176007	1
Caelo	Cloridrato de tetracaína	20004176008	9
Caelo	Cloridrato de tetracaína	20004176011	2
Caelo	Cloridrato de tetracaína	20004176012	3
Caelo	Cloridrato de tetracaína	20004176013	3
Caelo	Cloridrato de tetracaína	20004176015	4
Caelo	Cloridrato de tetracaína	20004176016	2
Caelo	Cloridrato de tetracaína	20004176019	3
Caelo	Cloridrato de tetracaína	20004176020	3
Caelo	Cloridrato de tetracaína	20004176021	1
Caelo	Cloridrato de tetracaína	2003053-01	1
Caelo	Cloridrato de tetracaína	2110008-01	1
Caelo	Cloridrato de tetracaína	22001496003	1
Caelo	Cloridrato de tetracaína	22001496004	4
Caelo	Cloridrato de tetracaína	2201496004	1
Caelo	Cloridrato de tetracaína	259/22	1
Caelo	Cloridrato de tetracaína	27111305	1
Caelo	Cloridrato de tetracaína	4176002	1
Caelo	Cloridrato de tetracaína	6093549	1
Caelo	Cloridrato de tetracaína	700216-0001	1
Caelo	Cloridrato de tetracaína	9070003	2
Caesar & Loretz GmbH...	Cloridrato de tetracaína	20004176003	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	22001496010	2
Caesar & Loretz GmbH/E	Cloridrato de tetracaína	20004176003	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	F10-3708006	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	TH0060219	1
Caesar & Loretz GmbH/Gehe	Cloridrato de tetracaína	190119001	1
Caesar & Loretz GmbH/Gehe	Cloridrato de tetracaína	1909024-02	2
Caesar & Loretz GmbH...	Cloridrato de tetracaína	19011908	2
Caesar & Loretz GmbH...	Cloridrato de tetracaína	18060614	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	18060621	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	20000156002	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	18060619	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	18060620	1
Caesar & Loretz GmbH...	Cloridrato de tetracaína	190119002	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	17G03-B07-351509	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	18060604	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	18060610	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	18060612	4
Caesar & Loretz GmbH	Cloridrato de tetracaína	18060619	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	18060621	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	190119001	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	190119002	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	190119003	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	19011901	5
Caesar & Loretz GmbH	Cloridrato de tetracaína	19011902	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	19011903	5
Caesar & Loretz GmbH	Cloridrato de tetracaína	19011906	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	19011907	5
Caesar & Loretz GmbH	Cloridrato de tetracaína	19011908	5
Caesar & Loretz GmbH	Cloridrato de tetracaína	20000156001	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	20000156002	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	20000156005	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	20000156006	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	20000156008	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176003	5
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176004	6
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176006	4
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176007	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176011	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176012	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176013	1
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176015	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176019	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	20004176020	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	22001496005	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	22001496010	2
Caesar & Loretz GmbH	Cloridrato de tetracaína	TH0100718	1
Caesar & Loretz	Cloridrato de tetracaína	1803001-01	1
Caesar & Loretz	Cloridrato de tetracaína	18060609	1
Caesar Loretz	Cloridrato de tetracaína	190229001	1
Caesar Loretz	Cloridrato de tetracaína	20000156006	1
Calo/AHD	Cloridrato de tetracaína	13155727	1
Ebert-Jacobi	Cloridrato de tetracaína	15K04-B03-328163	1
Ebert-Jacobi	Cloridrato de tetracaína	1612005-01	1
EuRho / Fiebig	Cloridrato de tetracaína	2010019-01	1
EuRho Anzag	Cloridrato de tetracaína	1207001-01	1
EuRho/ NOWEDA	Cloridrato de tetracaína	14G14-B08-300198	1
EuRho/ Noweda	Cloridrato de tetracaína	1803001-01	3
EuRho/ Phönix	Cloridrato de tetracaína	1612002-01	1
EuRho/	Cloridrato de tetracaína	1712012-01	2
EuRho/AHD	Cloridrato de tetracaína	1909024-01	1
EuRho/AHD	Cloridrato de tetracaína	2010019-02	1
EuRho/Alliance	Cloridrato de tetracaína	2001011-01	1
EuRho/Gehe	Cloridrato de tetracaína	1909024-01	1
EuRho/Noweda	Cloridrato de tetracaína	1706018-01	1
EuRho/Phoenix	Cloridrato de tetracaína	2110008-01	2
Eurho/Phönix	Cloridrato de tetracaína	2003053-01	1
Eurho/Phönix	Cloridrato de tetracaína	2010019-01	1
Eurho/Phönix	Cloridrato de tetracaína	211000801	1
EuRho/Sanacorp	Cloridrato de tetracaína	1909024-02	1
EuRho/Sanacorp	Cloridrato de tetracaína	2001011-01	1
EuRho	Cloridrato de tetracaína	1106035-01	2
EuRho	Cloridrato de tetracaína	1110010-01	2
EuRho	Cloridrato de tetracaína	1110010-02	1
EuRho	Cloridrato de tetracaína	1615I-02039	1
EuRho	Cloridrato de tetracaína	1712012-01	2
euRho	Cloridrato de tetracaína	1803001-01	1
EuRho	Cloridrato de tetracaína	1803001-01	1
EuRho	Cloridrato de tetracaína	1902015-01	1
EuRho	Cloridrato de tetracaína	1909024-02	2
EuRho	Cloridrato de tetracaína	2001011-01	1
EuRho	Cloridrato de tetracaína	2003053-01	2
EuRho	Cloridrato de tetracaína	2010019-01	2
EuRho	Cloridrato de tetracaína	2906009V-04	1
EuRho	Cloridrato de tetracaína	TH0060219	1
Euro CT Phönix	Cloridrato de tetracaína	1207001-02	1
Euro ETC / Phönix	Cloridrato de tetracaína	2110008-01	1
Euro OT/Phönix	Cloridrato de tetracaína	TH0030315	1
Euro OTC	Cloridrato de tetracaína		1
Euro OTC	Cloridrato de tetracaína	1011-012	1
Euro OTC	Cloridrato de tetracaína	10416THCL	1
Euro OTC	Cloridrato de tetracaína	1106035	1
Euro OTC	Cloridrato de tetracaína	1106035-01	1
Euro OTC	Cloridrato de tetracaína	1110010-01	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de tetracaína	1110010-02	6
Euro OTC	Cloridrato de tetracaína	11110010-02	1
Euro OTC	Cloridrato de tetracaína	1207001-01	8
Euro OTC	Cloridrato de tetracaína	1207001-02	8
Euro OTC	Cloridrato de tetracaína	130301201	1
Euro OTC	Cloridrato de tetracaína	1303012-01	21
Euro OTC	Cloridrato de tetracaína	1310006-01	18
Euro OTC	Cloridrato de tetracaína	1310006-02	2
Euro OTC	Cloridrato de tetracaína	13155710	4
Euro OTC	Cloridrato de tetracaína	13509155	1
Euro OTC	Cloridrato de tetracaína	1404026-02	1
Euro OTC	Cloridrato de tetracaína	1405025-01	1
Euro OTC	Cloridrato de tetracaína	140502601	1
Euro OTC	Cloridrato de tetracaína	1405026-01	18
Euro OTC	Cloridrato de tetracaína	1405026-02	1
Euro OTC	Cloridrato de tetracaína	1405026-04	6
Euro OTC	Cloridrato de tetracaína	1409026	1
Euro OTC	Cloridrato de tetracaína	14090-26	1
Euro OTC	Cloridrato de tetracaína	140902601	1
Euro OTC	Cloridrato de tetracaína	1409026-01	12
Euro OTC	Cloridrato de tetracaína	140902602	1
Euro OTC	Cloridrato de tetracaína	1409026-02	12
Euro OTC	Cloridrato de tetracaína	1411019	1
Euro OTC	Cloridrato de tetracaína	141101901	1
Euro OTC	Cloridrato de tetracaína	1411019-01	26
Euro OTC	Cloridrato de tetracaína	14G14-B08-300202	1
Euro OTC	Cloridrato de tetracaína	150604001	1
Euro OTC	Cloridrato de tetracaína	1506040-01	29
Euro OTC	Cloridrato de tetracaína	1506040-02	7
Euro OTC	Cloridrato de tetracaína	15120019-01	1
Euro OTC	Cloridrato de tetracaína	1512019-01	32
Euro OTC	Cloridrato de tetracaína	151-2019-01	1
Euro OTC	Cloridrato de tetracaína	1512019-02	2
Euro OTC	Cloridrato de tetracaína	1603026-01	1
Euro OTC	Cloridrato de tetracaína	1607031	1
Euro OTC	Cloridrato de tetracaína	1607031_01	1
Euro OTC	Cloridrato de tetracaína	160703101	2
Euro OTC	Cloridrato de tetracaína	1607031-01	39
Euro OTC	Cloridrato de tetracaína	1607032-01	1
Euro OTC	Cloridrato de tetracaína	161200501	4
Euro OTC	Cloridrato de tetracaína	1612005-01	38
Euro OTC	Cloridrato de tetracaína	1612005-015445	1
Euro OTC	Cloridrato de tetracaína	170323181	1
Euro OTC	Cloridrato de tetracaína	1706018-01	22
Euro OTC	Cloridrato de tetracaína	17081503	1
Euro OTC	Cloridrato de tetracaína	17114181	1
Euro OTC	Cloridrato de tetracaína	171201201	1
Euro OTC	Cloridrato de tetracaína	1712012-01	26
Euro OTC	Cloridrato de tetracaína	171212-01	1
Euro OTC	Cloridrato de tetracaína	18003001-01	1
Euro OTC	Cloridrato de tetracaína	1803001	1
Euro OTC	Cloridrato de tetracaína	180300101	10
Euro OTC	Cloridrato de tetracaína	1803001-01	48
Euro OTC	Cloridrato de tetracaína	1803001-1	1
Euro OTC	Cloridrato de tetracaína	180701701	2
Euro OTC	Cloridrato de tetracaína	1807017-01	8
Euro OTC	Cloridrato de tetracaína	18120006-01	1
Euro OTC	Cloridrato de tetracaína	1812006	2
Euro OTC	Cloridrato de tetracaína	181200601	2
Euro OTC	Cloridrato de tetracaína	1812006-01	33

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de tetracaína	18701701	1
Euro OTC	Cloridrato de tetracaína	1902012-01	2
Euro OTC	Cloridrato de tetracaína	1902015	1
Euro OTC	Cloridrato de tetracaína	1902015-01	33
Euro OTC	Cloridrato de tetracaína	1907007	1
Euro OTC	Cloridrato de tetracaína	1907007-01	14
Euro OTC	Cloridrato de tetracaína	1909024_01	1
Euro OTC	Cloridrato de tetracaína	1909024-0	1
Euro OTC	Cloridrato de tetracaína	190902401	1
Euro OTC	Cloridrato de tetracaína	1909024-01	74
Euro OTC	Cloridrato de tetracaína	1909024-02	17
Euro OTC	Cloridrato de tetracaína	1909024-21	1
Euro OTC	Cloridrato de tetracaína	19909024-01	1
Euro OTC	Cloridrato de tetracaína	20010019-01	1
Euro OTC	Cloridrato de tetracaína	2001011-01	16
Euro OTC	Cloridrato de tetracaína	2003053	1
Euro OTC	Cloridrato de tetracaína	200305301	1
Euro OTC	Cloridrato de tetracaína	2003053-01	39
Euro OTC	Cloridrato de tetracaína	2003053-02	4
Euro OTC	Cloridrato de tetracaína	2003053-03	1
Euro OTC	Cloridrato de tetracaína	2010010-01	1
Euro OTC	Cloridrato de tetracaína	2010019-01	45
Euro OTC	Cloridrato de tetracaína	2010019-02	14
Euro OTC	Cloridrato de tetracaína	2010091-01	1
Euro OTC	Cloridrato de tetracaína	201019-02	1
Euro OTC	Cloridrato de tetracaína	20160812-2	1
Euro OTC	Cloridrato de tetracaína	21071807	1
Euro OTC	Cloridrato de tetracaína	2110008-01	24
Euro OTC	Cloridrato de tetracaína	211008-01	1
Euro OTC	Cloridrato de tetracaína	2207015-01	5
Euro OTC	Cloridrato de tetracaína	2207015-02	1
Euro OTC	Cloridrato de tetracaína	24102014A	1
Euro OTC	Cloridrato de tetracaína	2906009V-03	1
Euro OTC	Cloridrato de tetracaína	3071716	1
Euro OTC	Cloridrato de tetracaína	3113M-02039	1
Euro OTC	Cloridrato de tetracaína	4811A-02039	1
Euro OTC	Cloridrato de tetracaína	5016Y-02039	1
Euro OTC	Cloridrato de tetracaína	6093547	1
Euro OTC	Cloridrato de tetracaína	Euro-OTC	1
Euro OTC	Cloridrato de tetracaína	TH0030315	1
Euro OTC	Cloridrato de tetracaína	TH00602019	1
Euro OTC	Cloridrato de tetracaína	TH0070816	1
Euro OTC	Cloridrato de tetracaína	TH0100718	2
Euro OTC	Cloridrato de tetracaína	TH0121219	2
Euro OTG Pharma	Cloridrato de tetracaína	1409026-02	1
Euro OTG/ AHD	Cloridrato de tetracaína	1706018-01	2
Euro OTG	Cloridrato de tetracaína	1207001-01	1
Euro/Phönix	Cloridrato de tetracaína	1506040-01	1
Euro	Cloridrato de tetracaína	1506040-01	1
euroct/gehe	Cloridrato de tetracaína	1405026-01	1
EuroTOC / Noweda	Cloridrato de tetracaína	131000601	2
EurRho/Noweda	Cloridrato de tetracaína	1712012-01	2
fag	Cloridrato de tetracaína	20G10-F07-373354	1
Fagreo / Sanacorp	Cloridrato de tetracaína	20A17F10370805	1
Fagro/Gehe	Cloridrato de tetracaína	16G28-B03-327368	2
Fagron	Cloridrato de tetracaína		1
Fagron	Cloridrato de tetracaína	10330837	1
Fagron	Cloridrato de tetracaína	10990834	3
Fagron	Cloridrato de tetracaína	10990837	3
Fagron	Cloridrato de tetracaína	10990841	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de tetracaína	10A29-N12	2
Fagron	Cloridrato de tetracaína	11/15-N12	1
Fagron	Cloridrato de tetracaína	11A31-N15	1
Fagron	Cloridrato de tetracaína	11C22-N04	1
Fagron	Cloridrato de tetracaína	12C22-N04	5
Fagron	Cloridrato de tetracaína	12H24-N05	12
Fagron	Cloridrato de tetracaína	12H24-N050696/1050	1
Fagron	Cloridrato de tetracaína	12H-N05	1
Fagron	Cloridrato de tetracaína	12K01-N04	7
Fagron	Cloridrato de tetracaína	1303012-01	1
Fagron	Cloridrato de tetracaína	13155711	1
Fagron	Cloridrato de tetracaína	13509149	2
Fagron	Cloridrato de tetracaína	13509155	1
Fagron	Cloridrato de tetracaína	13D11-N01	1
Fagron	Cloridrato de tetracaína	13D11-N07	12
Fagron	Cloridrato de tetracaína	13G02-N01	1
Fagron	Cloridrato de tetracaína	13H21-B02	2
Fagron	Cloridrato de tetracaína	13H21-B02-286558	3
Fagron	Cloridrato de tetracaína	13H21-B02-286559	1
Fagron	Cloridrato de tetracaína	13K25-B04	1
Fagron	Cloridrato de tetracaína	13k25-b04-290276	1
Fagron	Cloridrato de tetracaína	13K25-B04290276	1
Fagron	Cloridrato de tetracaína	13K25-B04-290276	3
Fagron	Cloridrato de tetracaína	13K25B04290277	1
Fagron	Cloridrato de tetracaína	13K25-B04-290278	1
Fagron	Cloridrato de tetracaína	13K25-Bo4-290276	1
Fagron	Cloridrato de tetracaína	1411019-01	2
Fagron	Cloridrato de tetracaína	1418-03-300199	1
Fagron	Cloridrato de tetracaína	14710369	1
Fagron	Cloridrato de tetracaína	14C18-B03	1
Fagron	Cloridrato de tetracaína	14C18-B03-293966	7
Fagron	Cloridrato de tetracaína	14C18-B03-293967	1
Fagron	Cloridrato de tetracaína	14C18-B03-300199	6
Fagron	Cloridrato de tetracaína	14C18-B03-300200	4
Fagron	Cloridrato de tetracaína	14C18-Bo3-300200	1
Fagron	Cloridrato de tetracaína	14c18d03300199	1
Fagron	Cloridrato de tetracaína	14G14B08300198	1
Fagron	Cloridrato de tetracaína	14G14-B08-300198	8
Fagron	Cloridrato de tetracaína	1506040-02	1
Fagron	Cloridrato de tetracaína	15A12B03308857	1
Fagron	Cloridrato de tetracaína	15A12-B03-308857	8
Fagron	Cloridrato de tetracaína	15H24-B03	3
Fagron	Cloridrato de tetracaína	15H24-B03-311450	6
Fagron	Cloridrato de tetracaína	15h24-b03-313594	1
Fagron	Cloridrato de tetracaína	15H24-B03-313594	6
Fagron	Cloridrato de tetracaína	15H24-B03-314243	1
Fagron	Cloridrato de tetracaína	15K04-B03	2
Fagron	Cloridrato de tetracaína	15K04-B03_322151	1
Fagron	Cloridrato de tetracaína	15K04-B03-318368	3
Fagron	Cloridrato de tetracaína	15K04B03318369	1
Fagron	Cloridrato de tetracaína	15K04-B03-318369	3
Fagron	Cloridrato de tetracaína	15K04-B03-321567	1
Fagron	Cloridrato de tetracaína	15K04-B03-321568	1
Fagron	Cloridrato de tetracaína	15K04-B03-322151	14
Fagron	Cloridrato de tetracaína	15K04-B03-328163	1
Fagron	Cloridrato de tetracaína	15K04-bo3-312151	1
Fagron	Cloridrato de tetracaína	1607031-01	1
Fagron	Cloridrato de tetracaína	16G28-B03	1
Fagron	Cloridrato de tetracaína	16G28-B03-327368	14
Fagron	Cloridrato de tetracaína	16G28-B03-327369	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de tetracaína	16G28-B03-328913	1
Fagron	Cloridrato de tetracaína	16G28-B03-330362	5
Fagron	Cloridrato de tetracaína	16G28-B03-330363	1
Fagron	Cloridrato de tetracaína	16G28-B03-332099	3
Fagron	Cloridrato de tetracaína	16G28-B03-334124	2
Fagron	Cloridrato de tetracaína	16G2-B03-327368	1
Fagron	Cloridrato de tetracaína	16G8-B03-327368	1
Fagron	Cloridrato de tetracaína	17114181	12
Fagron	Cloridrato de tetracaína	17G03_B07-351508	1
Fagron	Cloridrato de tetracaína	17G03-B07	8
Fagron	Cloridrato de tetracaína	17G03-B07-338538	7
Fagron	Cloridrato de tetracaína	17G03-B07-338539	4
Fagron	Cloridrato de tetracaína	17G03-B07-338540	1
Fagron	Cloridrato de tetracaína	17G03-B07-341319	1
Fagron	Cloridrato de tetracaína	17G03-B07-341853	4
Fagron	Cloridrato de tetracaína	17G03-B07-345008	7
Fagron	Cloridrato de tetracaína	17G03-B07-345009	3
Fagron	Cloridrato de tetracaína	17G03-B07-349367	5
Fagron	Cloridrato de tetracaína	17G03-B07-349368	2
Fagron	Cloridrato de tetracaína	17G03-B07-3515009	1
Fagron	Cloridrato de tetracaína	17G03-B07-351508	2
Fagron	Cloridrato de tetracaína	17G03-B07-351509	2
Fagron	Cloridrato de tetracaína	17G05-B04-341204	1
Fagron	Cloridrato de tetracaína	17Go3-B07-341853	1
Fagron	Cloridrato de tetracaína	1803001-01	1
Fagron	Cloridrato de tetracaína	1812006-01	1
Fagron	Cloridrato de tetracaína	18J03-B05	5
Fagron	Cloridrato de tetracaína	18J03-B05-356329	5
Fagron	Cloridrato de tetracaína	18J03-B05-356330	2
Fagron	Cloridrato de tetracaína	18J03-B05-358079	1
Fagron	Cloridrato de tetracaína	18J03B05358080	1
Fagron	Cloridrato de tetracaína	18J03-B05-358080	6
Fagron	Cloridrato de tetracaína	18J03-B05-359813	5
Fagron	Cloridrato de tetracaína	18J03-B05-359814	2
Fagron	Cloridrato de tetracaína	18J03-B05-359815	2
Fagron	Cloridrato de tetracaína	18J03-B05-361978	4
Fagron	Cloridrato de tetracaína	18J03-B05-361979	5
Fagron	Cloridrato de tetracaína	18J03-B05-362469	8
Fagron	Cloridrato de tetracaína	18J03-B05-362470	2
Fagron	Cloridrato de tetracaína	18J03-B05-362471	4
Fagron	Cloridrato de tetracaína	18J03-B05-58079	1
Fagron	Cloridrato de tetracaína	18j0-b05-358079	1
Fagron	Cloridrato de tetracaína	192021003	1
Fagron	Cloridrato de tetracaína	20A17-F10	3
Fagron	Cloridrato de tetracaína	20A17-F1008581264	1
Fagron	Cloridrato de tetracaína	20A17-F10-3708007	1
Fagron	Cloridrato de tetracaína	20A17-F10-370805	3
Fagron	Cloridrato de tetracaína	20A17-F10-370806	2
Fagron	Cloridrato de tetracaína	20A17-F10-370807	3
Fagron	Cloridrato de tetracaína	20G10-07-373352	1
Fagron	Cloridrato de tetracaína	20G10-F07	3
Fagron	Cloridrato de tetracaína	20G10-F07-372358	1
Fagron	Cloridrato de tetracaína	20G10-F07-373352	5
Fagron	Cloridrato de tetracaína	20G10F07373353	1
Fagron	Cloridrato de tetracaína	20G10-F07-373353	6
Fagron	Cloridrato de tetracaína	20G10-F07-373354	1
Fagron	Cloridrato de tetracaína	20G10-F07-374915	1
Fagron	Cloridrato de tetracaína	20G10-F07-374916	1
Fagron	Cloridrato de tetracaína	20L03-F02-377430	2
Fagron	Cloridrato de tetracaína	21120-B04-213603	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato de tetracaína	212131/221630-0002	1
Fagron	Cloridrato de tetracaína	218I-02039	1
Fagron	Cloridrato de tetracaína	21I20-B04-213603	2
Fagron	Cloridrato de tetracaína	21I20-B04-213604	4
Fagron	Cloridrato de tetracaína	21l20-B04-213604	1
Fagron	Cloridrato de tetracaína	221I20-B04-213603	1
Fagron	Cloridrato de tetracaína	2OA17-F10-370807	2
Fagron	Cloridrato de tetracaína	3413U02039	1
Fagron	Cloridrato de tetracaína	3913I-02039	1
Fagron	Cloridrato de tetracaína	4118A-02039	1
Fagron	Cloridrato de tetracaína	4313E-02039	1
Fagron	Cloridrato de tetracaína	6093547	2
Fagron	Cloridrato de tetracaína	6093549	1
Fagron	Cloridrato de tetracaína	715Q-02039	1
Fagron	Cloridrato de tetracaína	B05-3619708	2
Fagron	Cloridrato de tetracaína	F07-3733502	1
Fagron	Cloridrato de tetracaína	F10-3708005	1
Fagron	Cloridrato de tetracaína	F10-3708006	1
Fagron	Cloridrato de tetracaína	F10-3708007	1
Fagron	Cloridrato de tetracaína	TH0050520	2
Fagron	Cloridrato de tetracaína	TH0060721	1
Fagron	Cloridrato de tetracaína	TH0100718	6
Fargon / GEIBO	Cloridrato de tetracaína	21120-B04-213604	1
Fargon Services NL	Cloridrato de tetracaína	15K04-B03-322151	5
Fargon/AllianceH.	Cloridrato de tetracaína	17G03-B07-338538	1
Fargon/Noweda	Cloridrato de tetracaína	17G03-B07-345008	1
Fargron/ Sanacorp	Cloridrato de tetracaína	14C18-B03-300200	1
Fiebig/Calo	Cloridrato de tetracaína	17256704	1
Finze	Cloridrato de tetracaína	2906009-02	1
Gatt-Koller / Phoenix	Cloridrato de tetracaína	80/02140614	2
Gatt-Koller	Cloridrato de tetracaína	1803034	2
Gatt-Koller	Cloridrato de tetracaína	1900461	6
Gatt-Koller	Cloridrato de tetracaína	KNC1825J18	1
Gehe 07.07.2014	Cloridrato de tetracaína	13155706	1
Gehe amax	Cloridrato de tetracaína	1812006-01	1
gehe europharm	Cloridrato de tetracaína	201001901	1
Gehe	Cloridrato de tetracaína	1310006-01	1
Gehe	Cloridrato de tetracaína	13155711	2
Gehe	Cloridrato de tetracaína	15437119	1
Gehe	Cloridrato de tetracaína	15A12-B03-308857	1
Gehe	Cloridrato de tetracaína	15K04-B03-322151	1
GEHE	Cloridrato de tetracaína	1612005-01	1
GEHE	Cloridrato de tetracaína	1706018-01	1
GEHE	Cloridrato de tetracaína	17G03-B07-338540	1
Gehe	Cloridrato de tetracaína	1803001-01	1
GEHE	Cloridrato de tetracaína	18060602	2
GEHE	Cloridrato de tetracaína	18060614	2
Gehe	Cloridrato de tetracaína	1812006-01	1
Gehe	Cloridrato de tetracaína	1902015-01	1
Gehe	Cloridrato de tetracaína	1907007-01	1
Gehe	Cloridrato de tetracaína	1909024-01	1
Gehe	Cloridrato de tetracaína	200041	1
Gehe	Cloridrato de tetracaína	20004176008	1
Gehe	Cloridrato de tetracaína	2010019-02	1
Gehe	Cloridrato de tetracaína	2207015-02	1
Geibo/ Fargron	Cloridrato de tetracaína	15H24-B03-313594	1
Geibo/ Fargron	Cloridrato de tetracaína	17G03-B07-338538	1
Geibo	Cloridrato de tetracaína	2003053-01	1
Geibo	Cloridrato de tetracaína	22001496003	1
Geilenkirchen	Cloridrato de tetracaína	1812006-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Cloridrato de tetracaína	1902015-01	2
Geilenkirchen	Cloridrato de tetracaína	1909024-01	1
Gutenberg-Apotheke	Cloridrato de tetracaína	13D11-N07	1
Hänseler	Cloridrato de tetracaína		4
Hänseler	Cloridrato de tetracaína	2018060021	1
Jenne	Cloridrato de tetracaína	13D11-No7	1
Kehr	Cloridrato de tetracaína	22001496010	1
Lamotte/3	Cloridrato de tetracaína	13155720	1
Noveda	Cloridrato de tetracaína	12H24-N05	1
Noweda 06.02.19 EK:7,84	Cloridrato de tetracaína	1807017-01	1
Noweda Taucha	Cloridrato de tetracaína	2110008-01	1
Noweda/ BASF Pharma ...	Cloridrato de tetracaína	12H24-N05	1
Noweda	Cloridrato de tetracaína	1106035-01	2
Noweda	Cloridrato de tetracaína	120700-02	1
Noweda	Cloridrato de tetracaína	1310006-01	1
Noweda	Cloridrato de tetracaína	1405026-04	2
Noweda	Cloridrato de tetracaína	14G14-B08	1
Noweda	Cloridrato de tetracaína	17G03-B07-351508	2
Noweda	Cloridrato de tetracaína	1812006-01	1
Noweda	Cloridrato de tetracaína	18J03-B05-359814	1
Noweda	Cloridrato de tetracaína	19011908	1
Noweda	Cloridrato de tetracaína	1909024-1	1
Noweda	Cloridrato de tetracaína	20004176012	1
Noweda	Cloridrato de tetracaína	211008-01	2
Noweda	Cloridrato de tetracaína	22001496004	1
Noweda	Cloridrato de tetracaína	2207015-01	1
Noweda	Cloridrato de tetracaína	2207015-02	1
Noweda	Cloridrato de tetracaína	22J19-B01-221586	1
Noweda	Cloridrato de tetracaína	TH0050520	1
Nutra / Noweda	Cloridrato de tetracaína	1803001-01	1
Orgamol Pharma	Cloridrato de tetracaína	6093547	1
Pala	Cloridrato de tetracaína	18J03-B05-356329	1
Phoenix 04.11.16 Pho...	Cloridrato de tetracaína	1607031-01	1
Phoenix 27.07.2019 6,98EUR	Cloridrato de tetracaína	1712012-01	1
Phoenix am 30.04.2014	Cloridrato de tetracaína	1310006-01	1
Phoenix Goettin	Cloridrato de tetracaína	1409026-01	1
Phoenix	Cloridrato de tetracaína	15437104	2
Phoenix	Cloridrato de tetracaína	1803001-01	1
Phoenix	Cloridrato de tetracaína	20004176004	1
Phoenix	Cloridrato de tetracaína	2003053-01	2
Phoenix	Cloridrato de tetracaína	2010019-01	1
Phoenix	Cloridrato de tetracaína	2110008-01	1
Phoenix	Cloridrato de tetracaína	2207015-01	1
Phoenix	Cloridrato de tetracaína	3058	1
Phönix /euro	Cloridrato de tetracaína	2003053-01	1
Phönix	Cloridrato de tetracaína	130301201	1
Phönix	Cloridrato de tetracaína	1310006-01	1
Phönix	Cloridrato de tetracaína	1405026-01	1
PHÖNIX	Cloridrato de tetracaína	15437109	1
phönix	Cloridrato de tetracaína	15437121	1
Phönix	Cloridrato de tetracaína	1612005-01	1
Phönix	Cloridrato de tetracaína	171201201	1
Phönix	Cloridrato de tetracaína	1812006-01	1
Phönix	Cloridrato de tetracaína	1902015-01	1
Phönix	Cloridrato de tetracaína	1909024-01	1
PHÖNIX	Cloridrato de tetracaína	2003053-02	1
Phönix	Cloridrato de tetracaína	2010019-01	1
PHönix	Cloridrato de tetracaína	2010019-01	1
Phönix	Cloridrato de tetracaína	2015E-02039	1
Phönix	Cloridrato de tetracaína	2207015-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Cloridrato de tetracaína	2207015-03	1
Phönix	Cloridrato de tetracaína	22J19-B01-221586	1
Phönix	Cloridrato de tetracaína	2405009-01	3
Sana 20.12.17 7.99	Cloridrato de tetracaína	1612005-01	2
Sanacorp, 21.02.17, …	Cloridrato de tetracaína	1607031-01	1
Sanacorp/EuRho	Cloridrato de tetracaína	18060604	1
Sanacorp	Cloridrato de tetracaína	1207001-02	1
Sanacorp	Cloridrato de tetracaína	1303012-01	1
Sanacorp	Cloridrato de tetracaína	1409026-01	1
Sanacorp	Cloridrato de tetracaína	15/AKD1	1
Sanacorp	Cloridrato de tetracaína	17G03-B07-341318	1
Sanacorp	Cloridrato de tetracaína	17G03-B07-341853	1
Sanacorp	Cloridrato de tetracaína	1803001-01	2
Sanacorp	Cloridrato de tetracaína	19011903	2
Sanacorp	Cloridrato de tetracaína	1902015-01	1
Sanacorp	Cloridrato de tetracaína	2001011-01	1
Sanacorp	Cloridrato de tetracaína	20A17-F10	2
Sanacorp	Cloridrato de tetracaína	20A17-F10-370806	1
Sanacorp	Cloridrato de tetracaína	20G10-F07-373352	2
Sanacorp	Cloridrato de tetracaína	2110008-01	1
Sanacorp	Cloridrato de tetracaína	21I20-B04-213603	1
Sanacorp	Cloridrato de tetracaína	22001496004	1
sanacorp	Cloridrato de tetracaína	2207015-02	1
Sanacorp	Cloridrato de tetracaína	2207015-03	1
Sanacorp	Cloridrato de tetracaína	F07-3733502	1
Sino Phyto	Cloridrato de tetracaína	12019816	1
Synopharm/Anzag	Cloridrato de tetracaína	2712Q-02039	1
VDl 26.09.14 12,00 euro	Cloridrato de tetracaína	1405026-01	1
Venkata NA / Gehe	Cloridrato de tetracaína	190119002	2
Venkata Narayana / Gehe	Cloridrato de tetracaína	1907007-01	1
Venkata/Noweda	Cloridrato de tetracaína	TH00602019	1
Venkata/Noweda	Cloridrato de tetracaína	TH0060219	1
Venkata/phoenix	Cloridrato de tetracaína	TH0100718	1

- 233 979 spectra from 1515 *Apo-Ident* customers from a total of 48 878 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de tetracaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de tetracaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	345	0	152 617
Type B	0	910	0	201 174
Type C	0	2059	29	233 979

The substance/substance group *Cloridrato de tetracaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2609 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3407 %)
Type C	100.0000 % (> 99.9007 %)	98.6111 % (> 98.4674 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20924	21845	7,27	209,21
21845	21845	0,00	207,88
22285	22285	0,00	207,88
22912	22912	0,00	207,59
23162	21845	7,59	207,94
23163	21845	8,85	207,37
23500	21845	7,02	206,77
24141	24141	0,00	203,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de tetraciclina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20044-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de tetraciclina; Tetraciclina, cloridrato; Tetracyclini hydrochloridum

Special notes

When selecting the *Cloridrato de tetraciclina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de tetraciclina	8	7	185

Second-stage model

For differentiation of the substance/substance group *Cloridrato de tetraciclina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de tetraciclina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de clortetraciclina	54,75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de tetraciclina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de tetraciclina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de tetraciclina	13201303	21427	60	20130807
Caelo	Cloridrato de tetraciclina	13201303	21428	60	20130807
Caelo	Cloridrato de tetraciclina	161167	22468	60	20160504*
Caelo	Cloridrato de tetraciclina	15230712	22833	40	20150819
Caelo	Cloridrato de tetraciclina	20003996010	26301	30	20201127
Caelo	Cloridrato de tetraciclina	20003996010	26301SI	20	20201127
Euro OTC	Cloridrato de tetraciclina	1302012-01	21079	40	1411585
Euro OTC	Cloridrato de tetraciclina	1506012	21835	60	20150707*
Euro OTC	Cloridrato de tetraciclina	2004023	25279	40	20200721*
Euro OTC	Cloridrato de tetraciclina	2103015	25686	50	20210525*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Cloridrato de tetraciclina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 502 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 9 reference samples from the substance/substance group *Cloridrato de tetraciclina*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de tetraciclina	172858	23847	40
Caelo	Cloridrato de tetraciclina	181986	24256	40
Caelo	Cloridrato de tetraciclina	183083	24394	40
Euro OTC	Cloridrato de tetraciclina	1603026	22545	40
Euro OTC	Cloridrato de tetraciclina	1706020	23691	30
Euro OTC	Cloridrato de tetraciclina	1811031	24450	40
Euro OTC	Cloridrato de tetraciclina	2203017	26099	40
Euro OTC	Cloridrato de tetraciclina	2103015	25686SI†	10
Euro OTC	Cloridrato de tetraciclina	2203017	26099SI	40

- 201 764 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1032 spectra from 504 *Apo-Ident* customers from 190 batches from the substance/substance group *Cloridrato de tetraciclina*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 184 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de tetraciclina	21003348003	1
	Cloridrato de tetraciclina	21003348008	1
	Cloridrato de tetraciclina	21003348011	2
	Cloridrato de tetraciclina	21003348015	1
	Cloridrato de tetraciclina	21003348017	2
	Cloridrato de tetraciclina	2103015-02	4
	Cloridrato de tetraciclina	2203017-01	3
	Cloridrato de tetraciclina	23000427002	1
	Cloridrato de tetraciclina	23000427003	1
	Cloridrato de tetraciclina	23000427005	6
	Cloridrato de tetraciclina	23000427009	1
	Cloridrato de tetraciclina	24000509004	1
	Cloridrato de tetraciclina	24000509005	1
AHD	Cloridrato de tetraciclina	21003348003	1
AHD	Cloridrato de tetraciclina	23000427005	1
Aliance am 10.03.2014	Cloridrato de tetraciclina	1302012-02	1
Alliance Health 22.0...	Cloridrato de tetraciclina	13201307	1
Alliance Healthcare	Cloridrato de tetraciclina	192021008	1
Anzag/euRho	Cloridrato de tetraciclina		1
Bombastus	Cloridrato de tetraciclina	1204039-02	1
Bombastus	Cloridrato de tetraciclina	1603026-01	2
Bombastus	Cloridrato de tetraciclina	1811031-01	1
Caeli / Phönix	Cloridrato de tetraciclina	21003348002	1
Caelo	Cloridrato de tetraciclina	1017A-02378	1
Caelo	Cloridrato de tetraciclina	103201301	1
Caelo	Cloridrato de tetraciclina	111002901	1
Caelo	Cloridrato de tetraciclina	1160117	1
Caelo	Cloridrato de tetraciclina	1204039	2
Caelo	Cloridrato de tetraciclina	12138104	1
Caelo	Cloridrato de tetraciclina	12138106	2
Caelo	Cloridrato de tetraciclina	12353602	1
Caelo	Cloridrato de tetraciclina	12353603	6
Caelo	Cloridrato de tetraciclina	12353609	1
Caelo	Cloridrato de tetraciclina	12353612	1
Caelo	Cloridrato de tetraciclina	12353613	1
Caelo	Cloridrato de tetraciclina	1302012-01	1
Caelo	Cloridrato de tetraciclina	13201301	3
Caelo	Cloridrato de tetraciclina	13201302	1
Caelo	Cloridrato de tetraciclina	13201307	1
Caelo	Cloridrato de tetraciclina	13201309	2
Caelo	Cloridrato de tetraciclina	13F17-N03	1
Caelo	Cloridrato de tetraciclina	13L10B02296956	1
Caelo	Cloridrato de tetraciclina	1402030-01	1
Caelo	Cloridrato de tetraciclina	14080605	2
Caelo	Cloridrato de tetraciclina	14080606	4
Caelo	Cloridrato de tetraciclina	1412007-01	2
Caelo	Cloridrato de tetraciclina	1412007-03	3
Caelo	Cloridrato de tetraciclina	14364601	1
Caelo	Cloridrato de tetraciclina	14364604	3
Caelo	Cloridrato de tetraciclina	14364612	3
Caelo	Cloridrato de tetraciclina	14364614	1
Caelo	Cloridrato de tetraciclina	14364616	2
Caelo	Cloridrato de tetraciclina	14H06-B05-313591	1
Caelo	Cloridrato de tetraciclina	1506012-01	4
Caelo	Cloridrato de tetraciclina	151018-61	1
Caelo	Cloridrato de tetraciclina	15230703	4
Caelo	Cloridrato de tetraciclina	15230707	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de tetraciclina	15230711	1
Caelo	Cloridrato de tetraciclina	15230714	1
Caelo	Cloridrato de tetraciclina	15230715	5
Caelo	Cloridrato de tetraciclina	15230717	3
Caelo	Cloridrato de tetraciclina	15230720	3
Caelo	Cloridrato de tetraciclina	1603026-01	3
Caelo	Cloridrato de tetraciclina	1611617	1
Caelo	Cloridrato de tetraciclina	16116701	3
Caelo	Cloridrato de tetraciclina	16116704	1
Caelo	Cloridrato de tetraciclina	16116706	6
Caelo	Cloridrato de tetraciclina	16116708	1
Caelo	Cloridrato de tetraciclina	16116709	5
Caelo	Cloridrato de tetraciclina	16116714	2
Caelo	Cloridrato de tetraciclina	16116715	8
Caelo	Cloridrato de tetraciclina	16116720	2
Caelo	Cloridrato de tetraciclina	16116721	9
Caelo	Cloridrato de tetraciclina	166116709	1
Caelo	Cloridrato de tetraciclina	170602001	3
Caelo	Cloridrato de tetraciclina	1706020-01	6
Caelo	Cloridrato de tetraciclina	172855809	1
Caelo	Cloridrato de tetraciclina	17285801	12
Caelo	Cloridrato de tetraciclina	17285802	1
Caelo	Cloridrato de tetraciclina	17285803	9
Caelo	Cloridrato de tetraciclina	17285808	8
Caelo	Cloridrato de tetraciclina	17285809	5
Caelo	Cloridrato de tetraciclina	1811031/01	1
Caelo	Cloridrato de tetraciclina	1811031-01	2
Caelo	Cloridrato de tetraciclina	18198602	8
Caelo	Cloridrato de tetraciclina	18198603	9
Caelo	Cloridrato de tetraciclina	18198604	2
Caelo	Cloridrato de tetraciclina	18198608	12
Caelo	Cloridrato de tetraciclina	18198612	4
Caelo	Cloridrato de tetraciclina	18300213	1
Caelo	Cloridrato de tetraciclina	18308302	4
Caelo	Cloridrato de tetraciclina	18308303	2
Caelo	Cloridrato de tetraciclina	18308305	12
Caelo	Cloridrato de tetraciclina	18308306	2
Caelo	Cloridrato de tetraciclina	18308313	4
Caelo	Cloridrato de tetraciclina	18308314	3
Caelo	Cloridrato de tetraciclina	192021003	11
Caelo	Cloridrato de tetraciclina	192021004	11
Caelo	Cloridrato de tetraciclina	192021008	4
Caelo	Cloridrato de tetraciclina	192021011	26
Caelo	Cloridrato de tetraciclina	1920221011	1
Caelo	Cloridrato de tetraciclina	200003996008	1
Caelo	Cloridrato de tetraciclina	20001708003	2
Caelo	Cloridrato de tetraciclina	20001708004	8
Caelo	Cloridrato de tetraciclina	20001708005	5
Caelo	Cloridrato de tetraciclina	2000178003	1
Caelo	Cloridrato de tetraciclina	20003996002	4
Caelo	Cloridrato de tetraciclina	20003996003	9
Caelo	Cloridrato de tetraciclina	20003996004	4
Caelo	Cloridrato de tetraciclina	20003996006	6
Caelo	Cloridrato de tetraciclina	20003996010	6
Caelo	Cloridrato de tetraciclina	20003996011	4
Caelo	Cloridrato de tetraciclina	20003996017	1
Caelo	Cloridrato de tetraciclina	2000399606	1
Caelo	Cloridrato de tetraciclina	21003348002	4
Caelo	Cloridrato de tetraciclina	21003348003	7
Caelo	Cloridrato de tetraciclina	21003348004	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de tetraciclina	21003348008	1
Caelo	Cloridrato de tetraciclina	21003348011	9
Caelo	Cloridrato de tetraciclina	21003348033	1
Caelo	Cloridrato de tetraciclina	2714U-02378	1
Caelo	Cloridrato de tetraciclina	2883	1
Caelo	Cloridrato de tetraciclina	3314	1
Caelo	Cloridrato de tetraciclina	3341	1
Caelo	Cloridrato de tetraciclina	4012Q-02378	1
Caelo	Cloridrato de tetraciclina	4117I-02378	1
Caelo	Cloridrato de tetraciclina	4315I-02378	1
Caelo	Cloridrato de tetraciclina	5091202	1
Caelo	Cloridrato de tetraciclina	8682	1
Caelo	Cloridrato de tetraciclina	9248704	1
Caesar & Lorenz GmbH	Cloridrato de tetraciclina	18308312	1
Caesar & Lorenz GmbH	Cloridrato de tetraciclina	20001708005	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	18308312	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	192021010	2
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	20001708005	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	20003996008	2
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	21003348004	2
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	18308306	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	21003348011	1
Caesar & Loretz GmbH /E	Cloridrato de tetraciclina	18308305	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	20003996010	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	192021004	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	192021011	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	18308302	1
Caesar & Loretz GmbH/Kehr	Cloridrato de tetraciclina	18198612	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	18308313	1
Caesar & Loretz GmbH/Phoe	Cloridrato de tetraciclina	20003996004	1
Caesar & Loretz GmbH...	Cloridrato de tetraciclina	20001708004	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	102021011	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	18198612	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	18308302	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	18308303	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	18308305	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	18308306	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	18308313	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	192021003	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	192021008	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	192021011	6
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20001708004	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20001708005	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996002	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996003	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996004	3
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996006	4
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996010	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996011	3
Caesar & Loretz GmbH	Cloridrato de tetraciclina	20003996017	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	21003348002	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	21003348003	2
Caesar & Loretz GmbH	Cloridrato de tetraciclina	21003348010	1
Caesar & Loretz GmbH	Cloridrato de tetraciclina	21003348011	1
Caesar / Gehe	Cloridrato de tetraciclina	16116706	1
Celo/Kehr	Cloridrato de tetraciclina	13201307	1
EuRho / 107	Cloridrato de tetraciclina	1811031-01	1
EuRho/AHD	Cloridrato de tetraciclina		1
Eurho/Phoenix	Cloridrato de tetraciclina	1204039-02	1
EuRho/Phoenix	Cloridrato de tetraciclina	1811031-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Phoenix	Cloridrato de tetraciclina	2004023-01	1
Eurho/Phönix	Cloridrato de tetraciclina	1811031-01	2
EuRho/Sanacorp	Cloridrato de tetraciclina	2004023-01	1
EuRho	Cloridrato de tetraciclina	1302012-02	1
EuRho	Cloridrato de tetraciclina	1402030-02	1
EuRho	Cloridrato de tetraciclina	1811031-01	3
euRho	Cloridrato de tetraciclina	2004023-01	1
EuRho	Cloridrato de tetraciclina	2004023-01	1
EuRho	Cloridrato de tetraciclina	2203017-01	1
Euro OTC	Cloridrato de tetraciclina	100518-62	1
Euro OTC	Cloridrato de tetraciclina	1103003-01	1
Euro OTC	Cloridrato de tetraciclina	1110029-01	2
Euro OTC	Cloridrato de tetraciclina	12040390	1
Euro OTC	Cloridrato de tetraciclina	1204039-01	5
Euro OTC	Cloridrato de tetraciclina	120403902	1
Euro OTC	Cloridrato de tetraciclina	1204039-02	11
Euro OTC	Cloridrato de tetraciclina	1302012-01	7
Euro OTC	Cloridrato de tetraciclina	1302012-02	16
Euro OTC	Cloridrato de tetraciclina	13042015C	1
Euro OTC	Cloridrato de tetraciclina	140203001	1
Euro OTC	Cloridrato de tetraciclina	1402030-01	9
Euro OTC	Cloridrato de tetraciclina	1402030-02	9
Euro OTC	Cloridrato de tetraciclina	140410-62	1
Euro OTC	Cloridrato de tetraciclina	14120007-01	1
Euro OTC	Cloridrato de tetraciclina	141200701	1
Euro OTC	Cloridrato de tetraciclina	1412007-01	12
Euro OTC	Cloridrato de tetraciclina	1412007-03	12
Euro OTC	Cloridrato de tetraciclina	150601201	2
Euro OTC	Cloridrato de tetraciclina	1506012-01	29
Euro OTC	Cloridrato de tetraciclina	1506012-02	6
Euro OTC	Cloridrato de tetraciclina	1506012-02Eur	1
Euro OTC	Cloridrato de tetraciclina	151018-61	1
Euro OTC	Cloridrato de tetraciclina	160302	1
Euro OTC	Cloridrato de tetraciclina	1603026	2
Euro OTC	Cloridrato de tetraciclina	1603026_01	1
Euro OTC	Cloridrato de tetraciclina	160302601	1
Euro OTC	Cloridrato de tetraciclina	1603026-01	42
Euro OTC	Cloridrato de tetraciclina	16032026-01	1
Euro OTC	Cloridrato de tetraciclina	160621TCH	1
Euro OTC	Cloridrato de tetraciclina	1706020	2
Euro OTC	Cloridrato de tetraciclina	170602001	4
Euro OTC	Cloridrato de tetraciclina	1706020-01	66
Euro OTC	Cloridrato de tetraciclina	1706020-02	2
Euro OTC	Cloridrato de tetraciclina	17060201-01	1
Euro OTC	Cloridrato de tetraciclina	180306T/1412007-03	1
Euro OTC	Cloridrato de tetraciclina	1811031	2
Euro OTC	Cloridrato de tetraciclina	181103101	1
Euro OTC	Cloridrato de tetraciclina	1811031-01	81
Euro OTC	Cloridrato de tetraciclina	1811031-02	4
Euro OTC	Cloridrato de tetraciclina	18308314	1
Euro OTC	Cloridrato de tetraciclina	20004023-01	1
Euro OTC	Cloridrato de tetraciclina	2004023	3
Euro OTC	Cloridrato de tetraciclina	200402301	3
Euro OTC	Cloridrato de tetraciclina	2004023-01	54
Euro OTC	Cloridrato de tetraciclina	2004023-02	5
Euro OTC	Cloridrato de tetraciclina	210301501	1
Euro OTC	Cloridrato de tetraciclina	2103015-01	11
Euro OTC	Cloridrato de tetraciclina	2103015-02	1
Euro OTC	Cloridrato de tetraciclina	21031702	1
Euro OTC	Cloridrato de tetraciclina	21111404	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de tetraciclina	22(1706020-01)	1
Euro OTC	Cloridrato de tetraciclina	2203017-01	2
Euro OTC	Cloridrato de tetraciclina	2301001	1
Euro OTC	Cloridrato de tetraciclina	27101708	1
Euro OTC	Cloridrato de tetraciclina	28021315	1
Euro OTC	Cloridrato de tetraciclina	29052001	1
Euro OTC	Cloridrato de tetraciclina	411682	1
Euro OTC	Cloridrato de tetraciclina	80111031-01	1
Euro OTC	Cloridrato de tetraciclina	RetestCharge20219/3	1
Euro OTG/ AHD	Cloridrato de tetraciclina	1706020-01	1
EUro/AHD	Cloridrato de tetraciclina	1302012-01	1
Euro/Anzag	Cloridrato de tetraciclina	1603026-01	1
Euro/Jenne	Cloridrato de tetraciclina	2004023-01	2
EuRo/Noweda	Cloridrato de tetraciclina	1603026-01	1
EuRo/Noweda	Cloridrato de tetraciclina	1706020-01	1
euro/phönix	Cloridrato de tetraciclina	1506012-01	2
Euro/Phönix	Cloridrato de tetraciclina	200402302	1
Euro/Sanacorp	Cloridrato de tetraciclina	1811031-01	2
EuRoh/ Gehe	Cloridrato de tetraciclina	1811031	1
Europh/An	Cloridrato de tetraciclina	2004023-01	1
Europharm/Otto	Cloridrato de tetraciclina	1204039-01	1
Europharm/Otto	Cloridrato de tetraciclina	1204039-02	3
Fagron	Cloridrato de tetraciclina	12E10-N015	1
Fagron	Cloridrato de tetraciclina	12E10-N05	1
Fagron	Cloridrato de tetraciclina	12J15-N05	1
Fagron	Cloridrato de tetraciclina	13201301	1
Fagron	Cloridrato de tetraciclina	13F17-N03	4
Fagron	Cloridrato de tetraciclina	13J22-N04	1
Fagron	Cloridrato de tetraciclina	13L10-B02-294454	1
Fagron	Cloridrato de tetraciclina	13L10-B02-294455	2
Fagron	Cloridrato de tetraciclina	1402030-02	2
Fagron	Cloridrato de tetraciclina	14H06-B05	1
Fagron	Cloridrato de tetraciclina	14H06-B05-299498	1
Fagron	Cloridrato de tetraciclina	14H06-B05-303911	1
Fagron	Cloridrato de tetraciclina	14H06-B05-303912	7
Fagron	Cloridrato de tetraciclina	14H06-B05-311707	1
Fagron	Cloridrato de tetraciclina	14H06-B05-314870	1
Fagron	Cloridrato de tetraciclina	14H06-Bo5-303912	1
Fagron	Cloridrato de tetraciclina	1506012-01	1
Fagron	Cloridrato de tetraciclina	18308305	1
Fargon/Noweda	Cloridrato de tetraciclina	1811031-01	1
Gatt-Koller	Cloridrato de tetraciclina	1700729	1
Gehe Rostock	Cloridrato de tetraciclina	192021010	1
Gehe	Cloridrato de tetraciclina	1110029-01	1
Gehe	Cloridrato de tetraciclina	15230703	1
Gehe	Cloridrato de tetraciclina	16116706	1
Gehe	Cloridrato de tetraciclina	1706020-01	1
Gehe	Cloridrato de tetraciclina	18198603	1
GEHE	Cloridrato de tetraciclina	18198612	1
Gehe	Cloridrato de tetraciclina	2000178003	1
Gehe	Cloridrato de tetraciclina	2004023-01	1
Gehe	Cloridrato de tetraciclina	2103015-01	2
Gehe	Cloridrato de tetraciclina	2103015-02	1
GEHE	Cloridrato de tetraciclina	2203017-01	1
Hoff/ Noweda	Cloridrato de tetraciclina	14364604	1
Ichthyol/Phönix	Cloridrato de tetraciclina	1603026-01	1
Ichthyol-Gesellschaft	Cloridrato de tetraciclina	1603026-01	1
Jenne	Cloridrato de tetraciclina	1506012-02	1
Jenne	Cloridrato de tetraciclina	18198602	1
Jenne	Cloridrato de tetraciclina	21003348011	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr.22.04.2020	Cloridrato de tetraciclina	192021004	1
Ningxia / Caesar & L…	Cloridrato de tetraciclina	17285801	1
Ningxia Qiyuan Pharm…	Cloridrato de tetraciclina	21003348002	1
Ningxia Qiyuan Pharm…	Cloridrato de tetraciclina	1811031-01	1
ningxia	Cloridrato de tetraciclina	1412007-01	1
Ningxia	Cloridrato de tetraciclina	1603026-01	3
Noweda	Cloridrato de tetraciclina	13201307	1
Noweda	Cloridrato de tetraciclina	1412007-03	1
Noweda	Cloridrato de tetraciclina	1506012-01	1
Noweda	Cloridrato de tetraciclina	17285801	1
Noweda	Cloridrato de tetraciclina	17285802	1
Noweda	Cloridrato de tetraciclina	18198603	1
Noweda	Cloridrato de tetraciclina	21003348011	1
Noweda	Cloridrato de tetraciclina	2203017-01	1
Noweda	Cloridrato de tetraciclina	23000427003	2
Ph.Eur/Sanacorp	Cloridrato de tetraciclina	1811031-01	1
Phoenix	Cloridrato de tetraciclina	170602001	3
Phoenix	Cloridrato de tetraciclina	18198612	1
Phoenix	Cloridrato de tetraciclina	3428	1
Phönix Gotha	Cloridrato de tetraciclina	1302012-01	1
Phönix	Cloridrato de tetraciclina	16116715	1
PHÖNIX	Cloridrato de tetraciclina	16116721	1
Phönix	Cloridrato de tetraciclina	1706020-01	1
PHÖNIX	Cloridrato de tetraciclina	192021004	1
phönix	Cloridrato de tetraciclina	2103015-01	1
phönix	Cloridrato de tetraciclina	2203017-01	1
Röntgen	Cloridrato de tetraciclina	17285801	1
s. Protokol	Cloridrato de tetraciclina		1
Sanacorp	Cloridrato de tetraciclina	100403401	1
Sanacorp	Cloridrato de tetraciclina	1402030-01	1
Sanacorp	Cloridrato de tetraciclina	1603026-01	1
Sanacorp	Cloridrato de tetraciclina	192021011	1
Sanacorp	Cloridrato de tetraciclina	204023-01	1
Sanacorp	Cloridrato de tetraciclina	21003348008	1
Sanacorp	Cloridrato de tetraciclina	2203017-01	1
yinchuan Ningxia	Cloridrato de tetraciclina	1811031-01	1

- 235 035 spectra from 1515 *Apo-Ident* customers from a total of 49 074 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de tetraciclina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de tetraciclina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	320	0	201 764
Type C	0	1027	5	235 035

The substance/substance group *Cloridrato de tetraciclina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	99.5155 % (> 99.2248 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21079	21079	0,00	153,72
21427	21835	11,79	122,81
21428	21835	8,49	110,59
21835	21835	0,00	95,75
22468	22468	0,00	244,54
22833	25686	8,96	170,86
25279	25279	0,00	189,61
25686	25686	0,00	156,09
26301	21079	8,09	152,48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de vancomicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21748-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de vancomicina; Vancomicina, cloridrato; Vancomycini hydrochloridum

Special notes

When selecting the *Cloridrato de vancomicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de vancomicina	11	6	5

Second-stage model

For differentiation of the substance/substance group *Cloridrato de vancomicina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de vancomicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	49,09	–
Fosfato sódico de riboflavina hidratado	68,36	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de vancomicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de vancomicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Cloridrato de vancomicina	APHAP1609006EV	23532	40	AR-18-FG-000670-01
Euro OTC	Cloridrato de vancomicina	1407047-01	21748	60	AR-15-FG-008950-01
Euro OTC	Cloridrato de vancomicina	1506029	21826	60	AR-15-FG-009077-01
Euro OTC	Cloridrato de vancomicina	1610038	22878	40	20161208*
Euro OTC	Cloridrato de vancomicina	1810013	24325	40	20181029*
Euro OTC	Cloridrato de vancomicina	1908025	24854	40	20190923*
Euro OTC	Cloridrato de vancomicina	2002019	25269	40	20200629*
Euro OTC	Cloridrato de vancomicina	2203002	26048	40	20220419*
Euro OTC	Cloridrato de vancomicina	2402018	27294	40	20240710*
Fagron	Cloridrato de vancomicina	17I18-B08-340944	24010	40	20171109
Fagron	Cloridrato de vancomicina	18L18-B02-359948	24696	40	20190207

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Cloridrato de vancomicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 482 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 9 reference samples from the substance/substance group *Cloridrato de vancomicina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cloridrato de vancomicina	1604037	22891	40
Euro OTC	Cloridrato de vancomicina	1812005	24421	40
Euro OTC	Cloridrato de vancomicina	1902014	24492	40
Euro OTC	Cloridrato de vancomicina	2211001	26525	40
Fagron	Cloridrato de vancomicina	22G01-B07-221838	26383	40
Fagron	Cloridrato de vancomicina	23G06-B01-230986	26988	40
Euro OTC	Cloridrato de vancomicina	2203002	26048SI†	10
Euro OTC	Cloridrato de vancomicina	2211001	26525SI	20
Fagron	Cloridrato de vancomicina	22G01-B07-221838	26383SI	20

- 201 794 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 2 *Apo-Ident* customers from 5 batches from the substance/substance group *Cloridrato de vancomicina*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Cloridrato de vancomicina	1902014-01	2
Euro OTC	Cloridrato de vancomicina	2101015-01	1
Fagron	Cloridrato de vancomicina	20G16-F07	1
Fagron	Cloridrato de vancomicina	21G16-B01-217709	2
Fagron	Cloridrato de vancomicina	21G16-B01	1

- 236 060 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de vancomicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de vancomicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	290	0	201 794
Type C	0	5	2	236 060

The substance/substance group *Cloridrato de vancomicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21748	21748	0,00	110,62
21826	21826	0,00	89,33
22878	22878	0,00	101,61
23532	23532	0,00	88,17
24010	23532	27,60	93,54
24325	24325	0,00	88,94
24696	26048	11,63	102,04
24854	24854	0,00	114,10
25269	25269	0,00	102,24
26048	26048	0,00	108,49
27294	27294	0,00	96,26

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato de xilometazolina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20025-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato de xilometazolina; Xilometazolina, cloridrato; Xylometazolini hydrochloridum

Special notes

When selecting the *Cloridrato de xilometazolina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato de xilometazolina	7	5	82

Second-stage model

For differentiation of the substance/substance group *Cloridrato de xilometazolina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato de xilometazolina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aspartato de ornitina	64,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato de xilometazolina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato de xilometazolina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato de xilometazolina	13344901	21516	60	1501655
Caelo	Cloridrato de xilometazolina	13344901	21517	60	20131119
Caelo	Cloridrato de xilometazolina	16074211	23246	40	20160318
Fagron	Cloridrato de xilometazolina	13I18-B03-295481	21722	60	AR-15-FG-007785-01
Fagron	Cloridrato de xilometazolina	14K19-B05-305006	21927	60	20141128
Fagron	Cloridrato de xilometazolina	14K19-B05-305006	21927SI	60	20141128
Fagron	Cloridrato de xilometazolina	19B07-B02-373357	25735	40	20190408
Fagron	Cloridrato de xilometazolina	19B07-B02-373357	25735SI	40	20190408
Fagron	Cloridrato de xilometazolina	21K10-B04-215749	26060	40	20211207
Fagron	Cloridrato de xilometazolina	21K10-B04-215749	26060SI	40	20211207
Fagron	Cloridrato de xilometazolina	23L07-B05-227259	27047	40	20231213

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 540 spectra of 11 reference samples from the substance/substance group *Cloridrato de xilometazolina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 422 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 15 reference samples from the substance/substance group *Cloridrato de xilometazolina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato de xilometazolina	170739	23314	40
Caelo	Cloridrato de xilometazolina	173457	23832	40
Caelo	Cloridrato de xilometazolina	21000078002	25734	40
Caelo	Cloridrato de xilometazolina	22000302	26023	40
Caelo	Cloridrato de xilometazolina	24001236	27315	40
Caelo	Cloridrato de xilometazolina	13344901	21517SI†	60
Caelo	Cloridrato de xilometazolina	16074211	23246SI†	40
Caelo	Cloridrato de xilometazolina	170739	23314SI	40
Caelo	Cloridrato de xilometazolina	170739	23320	40
Caelo	Cloridrato de xilometazolina	170739	23320SI	40
Caelo	Cloridrato de xilometazolina	173457	23832SI	40
Caelo	Cloridrato de xilometazolina	21000078002	25734SI	40
Caelo	Cloridrato de xilometazolina	22000302	26023SI	40
Caelo	Cloridrato de xilometazolina	24001236	27315SI	40
Fagron	Cloridrato de xilometazolina	23L07-B05-227259	27047SI†	40

- 201 464 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

provided by the customer regarding manufacturer and batch number.

- 258 spectra from 172 *Apo-Ident* customers from 84 batches from the substance/substance group *Cloridrato de xilometazolina*.
- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato de xilometazolina	22000302001	2
	Cloridrato de xilometazolina	22000302006	1
	Cloridrato de xilometazolina	22000302010	1
	Cloridrato de xilometazolina	2200302004	1
	Cloridrato de xilometazolina	23002949001	1
	Cloridrato de xilometazolina	23002949004	1
Alliance	Cloridrato de xilometazolina	192761007	2
Alliance	Cloridrato de xilometazolina	22000302004	1
Anzag	Cloridrato de xilometazolina	12027911	1
Anzag	Cloridrato de xilometazolina	15037907	2
Caelo	Cloridrato de xilometazolina	10118821	2
Caelo	Cloridrato de xilometazolina	12027906	2
Caelo	Cloridrato de xilometazolina	12287201	2
Caelo	Cloridrato de xilometazolina	12287203	8
Caelo	Cloridrato de xilometazolina	12287204	2
Caelo	Cloridrato de xilometazolina	12287210	7
Caelo	Cloridrato de xilometazolina	12287212	2
Caelo	Cloridrato de xilometazolina	12287213	1
Caelo	Cloridrato de xilometazolina	13171202	10
Caelo	Cloridrato de xilometazolina	13171203	2
Caelo	Cloridrato de xilometazolina	13171205	1
Caelo	Cloridrato de xilometazolina	13344901	1
Caelo	Cloridrato de xilometazolina	13344908	1
Caelo	Cloridrato de xilometazolina	15037906	1
Caelo	Cloridrato de xilometazolina	15037907	4
Caelo	Cloridrato de xilometazolina	15037910	2
Caelo	Cloridrato de xilometazolina	15037912	1
Caelo	Cloridrato de xilometazolina	15292803	3
Caelo	Cloridrato de xilometazolina	15292804	5
Caelo	Cloridrato de xilometazolina	15292811	1
Caelo	Cloridrato de xilometazolina	15292812	2
Caelo	Cloridrato de xilometazolina	153037907	1
Caelo	Cloridrato de xilometazolina	160740209	1
Caelo	Cloridrato de xilometazolina	16074201	4
Caelo	Cloridrato de xilometazolina	16074202	2
Caelo	Cloridrato de xilometazolina	16074205	6
Caelo	Cloridrato de xilometazolina	16074209	8
Caelo	Cloridrato de xilometazolina	160742095416	1
Caelo	Cloridrato de xilometazolina	16074216	3
Caelo	Cloridrato de xilometazolina	16074217	3
Caelo	Cloridrato de xilometazolina	16322082	1
Caelo	Cloridrato de xilometazolina	1703902	1
Caelo	Cloridrato de xilometazolina	1703909	1
Caelo	Cloridrato de xilometazolina	17073902	3
Caelo	Cloridrato de xilometazolina	17073905	8
Caelo	Cloridrato de xilometazolina	17073908	1
Caelo	Cloridrato de xilometazolina	17073909	4
Caelo	Cloridrato de xilometazolina	17344512	1
Caelo	Cloridrato de xilometazolina	17345703	12
Caelo	Cloridrato de xilometazolina	17345706	2
Caelo	Cloridrato de xilometazolina	17345707	3
Caelo	Cloridrato de xilometazolina	17345708	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cloridrato de xilometazolina	17345712	4
Caelo	Cloridrato de xilometazolina	181102181	1
Caelo	Cloridrato de xilometazolina	192751007	1
Caelo	Cloridrato de xilometazolina	192761005	15
Caelo	Cloridrato de xilometazolina	192761007	7
Caelo	Cloridrato de xilometazolina	2031502	1
Caelo	Cloridrato de xilometazolina	21000078001	1
Caelo	Cloridrato de xilometazolina	21000078002	2
Caelo	Cloridrato de xilometazolina	21000078003	2
Caelo	Cloridrato de xilometazolina	21000078004	3
Caelo	Cloridrato de xilometazolina	2100078001	1
Caelo	Cloridrato de xilometazolina	2100078004	1
Caelo	Cloridrato de xilometazolina	21003217001	2
Caelo	Cloridrato de xilometazolina	21003217002	4
Caelo	Cloridrato de xilometazolina	2200030004	1
Caelo	Cloridrato de xilometazolina	22000302004	3
Caelo	Cloridrato de xilometazolina	22000302008	1
Caelo	Cloridrato de xilometazolina	220003302003	1
Caelo	Cloridrato de xilometazolina	23051820	1
Caelo	Cloridrato de xilometazolina	24111202	1
Caelo	Cloridrato de xilometazolina	9276404	1
Caelo	Cloridrato de xilometazolina	9278404	1
Caesar & Loretz GmbH...	Cloridrato de xilometazolina	21000078002	1
Caesar & Loretz GmbH...	Cloridrato de xilometazolina	21000078004	1
Caesar & Loretz GmbH...	Cloridrato de xilometazolina	17345712	1
Caesar & Loretz GmbH...	Cloridrato de xilometazolina	192761005	1
Caesar & Loretz GmbH...	Cloridrato de xilometazolina	17345710	1
Caesar & Loretz GmbH...	Cloridrato de xilometazolina	192761005	1
Caesar & Loretz GmbH	Cloridrato de xilometazolina	17073902	1
Caesar & Loretz GmbH	Cloridrato de xilometazolina	17345706	1
Caesar & Loretz GmbH	Cloridrato de xilometazolina	17345707	1
Caesar & Loretz GmbH	Cloridrato de xilometazolina	17345708	3
Caesar & Loretz GmbH	Cloridrato de xilometazolina	17345710	3
Caesar & Loretz GmbH	Cloridrato de xilometazolina	17345712	1
Caesar & Loretz GmbH	Cloridrato de xilometazolina	192761007	2
Caesar & Loretz GmbH	Cloridrato de xilometazolina	21000078001	2
Caesar & Loretz GmbH	Cloridrato de xilometazolina	21000078004	7
Caesar & Loretz GmbH	Cloridrato de xilometazolina	21003217002	4
Caesar & Loretz GmbH	Cloridrato de xilometazolina	22000302001	1
Celoa vdL	Cloridrato de xilometazolina	13171202	1
Fagron	Cloridrato de xilometazolina	10416XMHC	1
Fagron	Cloridrato de xilometazolina	12287210	1
Fagron	Cloridrato de xilometazolina	12G31-N01	1
Fagron	Cloridrato de xilometazolina	13171203	1
Fagron	Cloridrato de xilometazolina	1318-B03-295479	1
Fagron	Cloridrato de xilometazolina	13E06-N11	1
Fagron	Cloridrato de xilometazolina	13I09-N02	1
Fagron	Cloridrato de xilometazolina	15Jo6-B99-313751	1
Fagron	Cloridrato de xilometazolina	15K25-B07-318956	1
Fagron	Cloridrato de xilometazolina	21K10-B04-215749	1
Gehe	Cloridrato de xilometazolina	10118802	1
Gehe	Cloridrato de xilometazolina	16074201	1
GEHE	Cloridrato de xilometazolina	16074209	1
Gehe	Cloridrato de xilometazolina	17345703	1
Geilenkirchen	Cloridrato de xilometazolina	16074209	1
Geilenkirchen	Cloridrato de xilometazolina	17345708	1
InfectoPharm/Gehe	Cloridrato de xilometazolina	17345707	1
Nachprüfung	Cloridrato de xilometazolina	4317E-03337	1
Noweda	Cloridrato de xilometazolina	12027902	1
Noweda	Cloridrato de xilometazolina	12287203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Cloridrato de xilometazolina	17345708	1
Phönix	Cloridrato de xilometazolina	22000302003	1
Sanacorp	Cloridrato de xilometazolina	12027902	1
Sanacorp	Cloridrato de xilometazolina	15037906	1
Sanacorp	Cloridrato de xilometazolina	17345703	1
sanacorp	Cloridrato de xilometazolina	22000302003	1
Siegrfried Pharma Ch…	Cloridrato de xilometazolina	22000302008	1

- 235 809 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato de xilometazolina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato de xilometazolina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	620	0	201 464
Type C	0	257	1	235 809

The substance/substance group *Cloridrato de xilometazolina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.6124 % (> 98.4496 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21516	21516	0,00	82,99
21517	21516	5,39	84,11
21722	21722	0,00	86,68
21927	21722	7,81	87,86
23246	21722	6,42	85,05
25735	21722	10,97	86,48
26060	21722	8,77	86,21
27047	21722	19,61	87,93

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cloridrato do ácido 5-aminolevulínico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20371-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cloridrato do ácido 5-aminolevulínico; Ácido aminolevulínico, cloridrato; Acidum aminolaevulinicum hydrochloricum; Cloridrato do ácido aminolevulínico

Special notes

When selecting the *Cloridrato do ácido 5-aminolevulínico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cloridrato do ácido 5-aminolevulínico	7	6	83

Second-stage model

For differentiation of the substance/substance group *Cloridrato do ácido 5-aminolevulínico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cloridrato do ácido 5-aminolevulínico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	100,80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cloridrato do ácido 5-aminolevulínico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cloridrato do ácido 5-aminolevulínico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cloridrato do ácido 5-ami…	16357904	23208	40	1707616
Caelo	Cloridrato do ácido 5-ami…	16357904	23747	40	20170324
Caelo	Cloridrato do ácido 5-ami…	190219	24733	40	20190312*
Caelo	Cloridrato do ácido 5-ami…	192811002	25371	40	20191107
Caelo	Cloridrato do ácido 5-ami…	20004269	25645	40	20210202*
Fagron	Cloridrato do ácido 5-ami…	13K27-N02	21339	40	20131125
Fagron	Cloridrato do ácido 5-ami…	17A12-B07-332960	23403	40	20170131
Fagron	Cloridrato do ácido 5-ami…	17A12-B07-332960	23404	40	20170131
Fagron	Cloridrato do ácido 5-ami…	19K14-F02-366541	25372	40	20191209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Cloridrato do ácido 5-aminolevulínico*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 335 spectra of 11 reference samples from the substance/substance group *Cloridrato do ácido 5-aminolevulínico*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cloridrato do ácido 5-ami…	22003347	26505	40
Fagron	Cloridrato do ácido 5-ami…	18C16-B05-347714	24099	40
Fagron	Cloridrato do ácido 5-ami…	21G28-B05-216542	25843	50
Fagron	Cloridrato do ácido 5-ami…	21L14-B01-220727	26082	40
Fagron	Cloridrato do ácido 5-ami…	22B16-B03-218068	26297	40
Fagron	Cloridrato do ácido 5-ami…	23B17-B04-227315	26685	40
Caelo	Cloridrato do ácido 5-ami…	22003347	26505SI	20
Fagron	Cloridrato do ácido 5-ami…	21G28-B05-216542	25843SI	15
Fagron	Cloridrato do ácido 5-ami…	21L14-B01-220727	26082SI	10
Fagron	Cloridrato do ácido 5-ami…	22B16-B03-218068	26297SI	20
Fagron	Cloridrato do ácido 5-ami…	23B17-B04-227315	26685SI	20

- 201 749 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 116 spectra from 42 *Apo-Ident* customers from 87 batches from the substance/substance group *Cloridrato do ácido 5-aminolevulínico*.

- Among them are spectra of independent samples from 83 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cloridrato do ácido 5-ami...	13C-19-N07	1
	Cloridrato do ácido 5-ami...	23B17-B04-227317	1
Biosynth AG / Otto	Cloridrato do ácido 5-ami...	20563	1
Biosynth AG	Cloridrato do ácido 5-ami...	F05-3695208	1
Caelo	Cloridrato do ácido 5-ami...	11355616	1
Caelo	Cloridrato do ácido 5-ami...	12093205	2
Caelo	Cloridrato do ácido 5-ami...	12093208	1
Caelo	Cloridrato do ácido 5-ami...	13017402	1
Caelo	Cloridrato do ácido 5-ami...	13017403	1
Caelo	Cloridrato do ácido 5-ami...	13K27-N02	1
Caelo	Cloridrato do ácido 5-ami...	14145003	2
Caelo	Cloridrato do ácido 5-ami...	14145007	3
Caelo	Cloridrato do ácido 5-ami...	14145011	1
Caelo	Cloridrato do ácido 5-ami...	15254803	1
Caelo	Cloridrato do ácido 5-ami...	16357902	1
Caelo	Cloridrato do ácido 5-ami...	16357910	1
Caelo	Cloridrato do ácido 5-ami...	18026102	1
Caelo	Cloridrato do ácido 5-ami...	18C16-B05-347711	1
Caelo	Cloridrato do ácido 5-ami...	18C16-B05-37711	1
Caelo	Cloridrato do ácido 5-ami...	19281105	1
Caeolo	Cloridrato do ácido 5-ami...	15254803	1
Caesar & Loretz GmbH	Cloridrato do ácido 5-ami...	192811002	1
Caesar & Loretz GmbH	Cloridrato do ácido 5-ami...	20004269005	1
Caesar & Loretz GmbH	Cloridrato do ácido 5-ami...	22003347002	1
Euro OTC	Cloridrato do ácido 5-ami...	18L03-B01-357231	1
Fagron	Cloridrato do ácido 5-ami...	11I30-N01	1
Fagron	Cloridrato do ácido 5-ami...	12c23-n05	1
Fagron	Cloridrato do ácido 5-ami...	12H20-N01	1
Fagron	Cloridrato do ácido 5-ami...	12K26-N05	1
Fagron	Cloridrato do ácido 5-ami...	13C19-N05	3
Fagron	Cloridrato do ácido 5-ami...	13G18-B06-355728	1
Fagron	Cloridrato do ácido 5-ami...	13H13-N07	2
Fagron	Cloridrato do ácido 5-ami...	13J29-N03	2
Fagron	Cloridrato do ácido 5-ami...	13K27-N02	2
Fagron	Cloridrato do ácido 5-ami...	14802	1
Fagron	Cloridrato do ácido 5-ami...	14K04-B01-297971	2
Fagron	Cloridrato do ácido 5-ami...	14K13-B01	1
Fagron	Cloridrato do ácido 5-ami...	15C06-B02-305245	1
Fagron	Cloridrato do ácido 5-ami...	15J23-B06	1
Fagron	Cloridrato do ácido 5-ami...	15J23-B06-314284	1
Fagron	Cloridrato do ácido 5-ami...	16A11-B02	1
Fagron	Cloridrato do ácido 5-ami...	16A11-B02-316734	1
Fagron	Cloridrato do ácido 5-ami...	16A11-B02-317459	3
Fagron	Cloridrato do ácido 5-ami...	16A11-B02-318406	1
Fagron	Cloridrato do ácido 5-ami...	16E17-B08-324962	2
Fagron	Cloridrato do ácido 5-ami...	16G27-B10	1
Fagron	Cloridrato do ácido 5-ami...	16I12-B06	1
Fagron	Cloridrato do ácido 5-ami...	16I12-B06-326185	1
Fagron	Cloridrato do ácido 5-ami...	16K17-B09-328197	1
Fagron	Cloridrato do ácido 5-ami...	16K17-B09-330371	1
Fagron	Cloridrato do ácido 5-ami...	17/22-B02-342555	1
Fagron	Cloridrato do ácido 5-ami...	1701-b05-342090	1
Fagron	Cloridrato do ácido 5-ami...	17A12-B07-331744	1
Fagron	Cloridrato do ácido 5-ami...	17A12-B07-331745	1
Fagron	Cloridrato do ácido 5-ami...	17F01-B05-338204	1
Fagron	Cloridrato do ácido 5-ami...	17F01-B06_337165	1
Fagron	Cloridrato do ácido 5-ami...	17F01-B06-337163	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloridrato do ácido 5-ami…	17F01-B06-337164	2
Fagron	Cloridrato do ácido 5-ami…	17I22-B02	3
Fagron	Cloridrato do ácido 5-ami…	17I22-B02-343410	1
Fagron	Cloridrato do ácido 5-ami…	17I22-B02-343411	1
Fagron	Cloridrato do ácido 5-ami…	17L18-B05-344673	1
Fagron	Cloridrato do ácido 5-ami…	17l22-B02-343410	1
Fagron	Cloridrato do ácido 5-ami…	18C16-B05	4
Fagron	Cloridrato do ácido 5-ami…	18C16-B05-347714	1
Fagron	Cloridrato do ácido 5-ami…	18D10-B02-361711	1
Fagron	Cloridrato do ácido 5-ami…	18D17-B02349681	1
Fagron	Cloridrato do ácido 5-ami…	18G13-806-352897	1
Fagron	Cloridrato do ácido 5-ami…	18G13-B06	2
Fagron	Cloridrato do ácido 5-ami…	18G13-B06-355728	1
Fagron	Cloridrato do ácido 5-ami…	18L03-B01	1
Fagron	Cloridrato do ácido 5-ami…	18L03-B01-360101	1
Fagron	Cloridrato do ácido 5-ami…	19G31-B02	5
Fagron	Cloridrato do ácido 5-ami…	19G31-B02-363475	1
Fagron	Cloridrato do ácido 5-ami…	19G31-B02-364671	1
Fagron	Cloridrato do ácido 5-ami…	19G31-B02-364672	1
Fagron	Cloridrato do ácido 5-ami…	19G31-B02-36473	1
Fagron	Cloridrato do ácido 5-ami…	19K14-F02-366541	1
Fagron	Cloridrato do ácido 5-ami…	19K14-F02-366544	1
Fagron	Cloridrato do ácido 5-ami…	19K14-F02-368326	1
Fagron	Cloridrato do ácido 5-ami…	20A29-F05-367867	1
Fagron	Cloridrato do ácido 5-ami…	20A29-F05-369528	1
Fagron	Cloridrato do ácido 5-ami…	20F04-F01-371115	1
Fagron	Cloridrato do ácido 5-ami…	20F04-F02-371121	1
Fagron	Cloridrato do ácido 5-ami…	21G28-B05-213714	2
Fagron	Cloridrato do ácido 5-ami…	22H03-B02-225921	1
Fagron	Cloridrato do ácido 5-ami…	23B17-B04-227317	1
Fagron	Cloridrato do ácido 5-ami…	25414	1
Fagron	Cloridrato do ácido 5-ami…	7447	1
Fiebig	Cloridrato do ácido 5-ami…	18c16-b05-347711	1

- 235 951 spectra from 1515 *Apo-Ident* customers from a total of 49 172 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cloridrato do ácido 5-aminolevulínico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cloridrato do ácido 5-aminolevulínico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	335	0	201 749
Type C	0	114	2	235 951

The substance/substance group *Cloridrato do ácido 5-aminolevulínico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2090 %)
Type C	100.0000 % (> 99.9007 %)	98.2759 % (> 95.6897 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21339	23208	55,78	127,69
23208	23208	0,00	127,97
23403	23208	47,00	126,23
23404	23208	39,21	127,16
23747	23208	6,01	127,92
24733	24733	0,00	123,82
25371	23208	37,98	129,79
25372	23208	45,59	126,98
25645	25645	0,00	127,15

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clorocresol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20185-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clorocresol; Chlorocresolum

Special notes

When selecting the *Clorocresol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clorocresol	5	2	16

Second-stage model

For differentiation of the substance/substance group *Clorocresol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clorocresol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	89,04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clorocresol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clorocresol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clorocresol	13275106	21512	60	20130828
Caelo	Clorocresol	13275106	21513	60	20130828
Caelo	Clorocresol	163378	23357	40	20170124*
Caelo	Clorocresol	182523	24406	40	20180919*
Caelo	Clorocresol	190837	24717	40	20190508*
Caelo	Clorocresol	21004157	27127	40	20220303*
Caelo	Clorocresol	21004157	27127SI	20	20220303*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Clorocresol*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 662 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Clorocresol*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clorocresol	15114107	23411	40
Caelo	Clorocresol	181360	24050	40

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 36 spectra from 27 *Apo-Ident* customers from 16 batches from the substance/substance group *Clorocresol*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clorocresol	22002861005	1
Caelo	Clorocresol	10145239	3
Caelo	Clorocresol	12111013	2
Caelo	Clorocresol	12111017	2
Caelo	Clorocresol	13275117	1
Caelo	Clorocresol	15114107	1
Caelo	Clorocresol	18027101	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clorocresol	18027110	2
Caelo	Clorocresol	18136006	6
Caelo	Clorocresol	20004363020	1
Caelo	Clorocresol	20101808	1
Caelo	Clorocresol	2041513	1
Caelo	Clorocresol	23415422	1
Caelo	Clorocresol	4613M-01260	1
Caelo	Clorocresol	7061304	1
Caesar & Loretz GmbH/Gehe	Clorocresol	18136006	1
Caesar & Loretz GmbH…	Clorocresol	18027101	1
Caesar & Loretz GmbH	Clorocresol	12111017	1
Caesar & Loretz GmbH	Clorocresol	18136006	2
Noweda	Clorocresol	12111017	1
Noweda	Clorocresol	22002861005	1
Spangropharm	Clorocresol		1

- 236 031 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clorocresol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clorocresol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	80	0	202 004
Type C	0	36	0	236 031

The substance/substance group *Clorocresol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 83.3333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21512	24406	15,85	163,94
21513	27127	12,60	167,64
23357	23357	0,00	153,35
24406	24406	0,00	170,49
24717	24717	0,00	156,17
27127	27127	0,00	168,10

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clotrimazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20000-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clotrimazol; Clotrimazolum

Special notes

When selecting the *Clotrimazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clotrimazol	12	15	881

Second-stage model

For differentiation of the substance/substance group *Clotrimazol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clotrimazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Bifonazol	42,54	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clotrimazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clotrimazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clotrimazol	13184113	21087	40	20130614
Caelo	Clotrimazol	13224204	21114	40	20130815
Caelo	Clotrimazol	13224220	21352	40	20130815
Caelo	Clotrimazol	13224220	21353	40	20130815
Caelo	Clotrimazol	153956	23791	40	20151215*
Caelo	Clotrimazol	21000121	25649	40	20210330*
Caelo	Clotrimazol	21000123	25656	40	20210330*
Euro OTC	Clotrimazol	1306036-01	21207	40	20130823
Euro OTC	Clotrimazol	1510003	22229	60	20151111*
Fagron	Clotrimazol	12I21-N01	20794	40	20120322
Fagron	Clotrimazol	14B05-B36	21259	40	20140225
Fagron	Clotrimazol	14C04-B31	21264	40	20140319
Fagron	Clotrimazol	22A21-B02-217361	26137	40	20220411

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 13 reference samples from the substance/substance group *Clotrimazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 422 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 640 spectra of 18 reference samples from the substance/substance group *Clotrimazol*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clotrimazol	12320815	20861	30
Caelo	Clotrimazol	171116	23322	40
Caelo	Clotrimazol	17111616	23781	40
Caelo	Clotrimazol	190161	24512	40
Caelo	Clotrimazol	190162	24517	40
Caelo	Clotrimazol	21004117	26001	40
Caelo	Clotrimazol	23001597	26834	40
Euro OTC	Clotrimazol	1607046	22793	40
Euro OTC	Clotrimazol	1703028	23129	40
Euro OTC	Clotrimazol	1808028	24298	40
Euro OTC	Clotrimazol	1902004	24461	40
Euro OTC	Clotrimazol	2007033	25300	40
Euro OTC	Clotrimazol	2103024	25672	40
Euro OTC	Clotrimazol	2301055	26582	40
Euro OTC	Clotrimazol	2406013	27400	40
Caelo	Clotrimazol	21004117	26001SI	10
Euro OTC	Clotrimazol	2301055	26582SI	20
Fagron	Clotrimazol	22A21-B02-217361	26137SI†	20

- 201 444 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6943 spectra from 1318 *Apo-Ident* customers from 933 batches from the substance/substance group *Clotrimazol*.
- Among them are spectra of independent samples from 878 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clotrimazol	1306036-01	1
	Clotrimazol	14C04-B30-291661	1
	Clotrimazol	20H26-F05	1
	Clotrimazol	20H26-F05-373737	1
	Clotrimazol	20H26-F05-373738	1
	Clotrimazol	21000123010	1
	Clotrimazol	2100411016	1
	Clotrimazol	210041160007	1
	Clotrimazol	21004116005	5
	Clotrimazol	21004116007	9
	Clotrimazol	21004116008	2
	Clotrimazol	21004116012	1
	Clotrimazol	21004116013	3
	Clotrimazol	21004116014	21
	Clotrimazol	21004116016	4
	Clotrimazol	21004116017	1
	Clotrimazol	21004117004	1
	Clotrimazol	21004117005	1
	Clotrimazol	2100411701	1
	Clotrimazol	21004117011	1
	Clotrimazol	21004117013	1
	Clotrimazol	21004117016	2
	Clotrimazol	21004117017	7
	Clotrimazol	21004117018	15
	Clotrimazol	21004117019	6
	Clotrimazol	21004117022	9
	Clotrimazol	21004117023	2
	Clotrimazol	2100416016	1
	Clotrimazol	2103024-01	1
	Clotrimazol	2103024-02	8
	Clotrimazol	2103024-03	4
	Clotrimazol	214116014	1
	Clotrimazol	21D22-B03	1
	Clotrimazol	21D22-B03-217092	2
	Clotrimazol	21i24_b11_213292	1
	Clotrimazol	21I24-B11	1
	Clotrimazol	21I24-B11-213292	2
	Clotrimazol	22A21-B02-217361	1
	Clotrimazol	22A21-B02-217510	1
	Clotrimazol	22A21-B02-221730	2
	Clotrimazol	22A21-B02-221731	1
	Clotrimazol	22G29-B05-228695	1
	Clotrimazol	23001596002	19

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Clotrimazol	23001596003	4
	Clotrimazol	23001596008	3
	Clotrimazol	23001596009	5
	Clotrimazol	23001596010	3
	Clotrimazol	23003390001	1
	Clotrimazol	23003390004	1
	Clotrimazol	23003390005	1
	Clotrimazol	2301055_01	1
	Clotrimazol	23010550-01	1
	Clotrimazol	2301055-01	17
	Clotrimazol	2301055-02	10
	Clotrimazol	23D11-B01-228693	1
	Clotrimazol	23H09-B07-230826	1
	Clotrimazol	B11-2186308	1
	Clotrimazol	caelo	1
	Clotrimazol	HCZ20120	1
A.H.D.	Clotrimazol	14337801	1
AHC	Clotrimazol	23001596009	1
AHD 27.10 Ek.7,07	Clotrimazol	1607046	1
AHD/EuRho	Clotrimazol	1902004-01	1
AHD/Euro	Clotrimazol	1808028-02	1
AHD/Hedinger	Clotrimazol	14337807	1
AHD	Clotrimazol	13184105	1
AHD	Clotrimazol	14144914	1
AHD	Clotrimazol	16J07-B02-335773	1
AHD	Clotrimazol	16J07-B02-344817	1
AHD	Clotrimazol	1703028-03	1
AHD	Clotrimazol	1808028-01	1
AHD	Clotrimazol	18A18-B05-352114	1
AHD	Clotrimazol	190200-02	2
AHD	Clotrimazol	1902004-01	1
AHD	Clotrimazol	19B14-B01-359538	1
AHD	Clotrimazol	21004116008	1
AHD	Clotrimazol	21004116016	1
AHD	Clotrimazol	21004117023	1
AHD	Clotrimazol	2103024-02	1
AHD	Clotrimazol	2103024-03	1
AHD	Clotrimazol	22A21-B02-221730	1
AHD	Clotrimazol	23H09-B07-235135	1
Alliance Healthcare	Clotrimazol	1309034-01	1
Alliance Healthcare	Clotrimazol	18147216	1
Alliance Healthcare	Clotrimazol	21004117001	1
Alliance Healthcare	Clotrimazol	AP1510003-01C	1
Alliance	Clotrimazol	21004117011	1
Allianz Healthcare	Clotrimazol	18g10-b06-355382	1
Amoli / Gehe	Clotrimazol	CLT/1505/0016B	2
Amoli Organics Plot ...	Clotrimazol	17J25-Bo6-349161	1
Anzag	Clotrimazol	14C04-B30-2916618	1
Anzag	Clotrimazol	15395610	1
Anzag	Clotrimazol	15G14-B06	1
Anzag	Clotrimazol	1703028-01	1
Anzag	Clotrimazol	2007033-02	1
Anzag	Clotrimazol	2301055-04	1
apo ident	Clotrimazol	1607046-02	1
apo-ident	Clotrimazol	1902004-03	1
ApoIdent	Clotrimazol	2103024-1	1
Apo-klent	Clotrimazol	2103024-02	1
apomix	Clotrimazol	14B05-B36	1
apomix	Clotrimazol	15G14-B05-311100	1
apomix	Clotrimazol	15G14-B05-311103	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Clotrimazol	1703/0016CC	1
Audor Pharma	Clotrimazol	1703028-02	1
Audor Pharma	Clotrimazol	2007033-01	1
Audor Pharma	Clotrimazol	2007033-02	1
Audor Pharma	Clotrimazol	AP1306036-01C	1
Audor Pharma	Clotrimazol	APCL/1703/0016C	1
Audor Pharma	Clotrimazol	APCLT/1703/0016C	2
Audor Pharma	Clotrimazol	APCLT/1703/0016CC	4
Beiersdorf	Clotrimazol	15395611	1
Bombastus	Clotrimazol	1210039/02	1
Bombastus	Clotrimazol	12320815	1
Bombastus	Clotrimazol	14337817	1
Bombastus	Clotrimazol	1607046-01	2
Bombastus	Clotrimazol	17360203	1
Bombastus	Clotrimazol	18147211	1
Bombastus	Clotrimazol	Validierungsmessung	1
Caeelo / Gehe	Clotrimazol	18147211	1
cael	Clotrimazol	19016208	2
Caello/Anzag	Clotrimazol	14337815	1
Caelo	Clotrimazol		10
Caelo	Clotrimazol	10147203	1
Caelo	Clotrimazol	10247328	3
Caelo	Clotrimazol	1070716	1
Caelo	Clotrimazol	108/AKD1	1
Caelo	Clotrimazol	11/22-N10	1
Caelo	Clotrimazol	1105014-02	1
Caelo	Clotrimazol	11081201	1
Caelo	Clotrimazol	11305506	2
Caelo	Clotrimazol	11305507	1
Caelo	Clotrimazol	11305511	1
Caelo	Clotrimazol	11305513	8
Caelo	Clotrimazol	1150817/16234512	1
Caelo	Clotrimazol	1170717	1
Caelo	Clotrimazol	11-K21-N19	1
Caelo	Clotrimazol	1210030-02	1
Caelo	Clotrimazol	1210039-01	1
Caelo	Clotrimazol	12159902	11
Caelo	Clotrimazol	12159904	2
Caelo	Clotrimazol	12159911	2
Caelo	Clotrimazol	12159913	9
Caelo	Clotrimazol	12159916	6
Caelo	Clotrimazol	12320805	4
Caelo	Clotrimazol	12320806	5
Caelo	Clotrimazol	12320807	4
Caelo	Clotrimazol	12320808	11
Caelo	Clotrimazol	12320809	4
Caelo	Clotrimazol	12320813	3
Caelo	Clotrimazol	12320814	9
Caelo	Clotrimazol	12320815	1
Caelo	Clotrimazol	1234567	1
Caelo	Clotrimazol	1259913	1
Caelo	Clotrimazol	12B27-N05	2
Caelo	Clotrimazol	12E02-N12	2
Caelo	Clotrimazol	12E30-N07	1
Caelo	Clotrimazol	12I21-N04	1
Caelo	Clotrimazol	1306036	1
Caelo	Clotrimazol	130603601	1
Caelo	Clotrimazol	1306036-01	4
Caelo	Clotrimazol	1309034-02	3
Caelo	Clotrimazol	1309034-C1	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	13148007	1
Caelo	Clotrimazol	13184103	10
Caelo	Clotrimazol	13184105	13
Caelo	Clotrimazol	13184111	7
Caelo	Clotrimazol	131841111	1
Caelo	Clotrimazol	13184113	2
Caelo	Clotrimazol	132234216	1
Caelo	Clotrimazol	1322401	1
Caelo	Clotrimazol	13224201	21
Caelo	Clotrimazol	13224204	2
Caelo	Clotrimazol	13224210	11
Caelo	Clotrimazol	13224211	5
Caelo	Clotrimazol	13224212	8
Caelo	Clotrimazol	13224214	9
Caelo	Clotrimazol	13224215	3
Caelo	Clotrimazol	13224216	9
Caelo	Clotrimazol	13224217	9
Caelo	Clotrimazol	13224218	12
Caelo	Clotrimazol	13224219	7
Caelo	Clotrimazol	13224220	6
Caelo	Clotrimazol	13224221	2
Caelo	Clotrimazol	13224225	2
Caelo	Clotrimazol	132243218	1
Caelo	Clotrimazol	13324204	1
Caelo	Clotrimazol	1409027-02	2
Caelo	Clotrimazol	1409027-03	3
Caelo	Clotrimazol	1409027-04	1
Caelo	Clotrimazol	14101716	1
Caelo	Clotrimazol	141104C	1
Caelo	Clotrimazol	14144905	17
Caelo	Clotrimazol	14144911	13
Caelo	Clotrimazol	14144912	2
Caelo	Clotrimazol	14144913	2
Caelo	Clotrimazol	14144914	8
Caelo	Clotrimazol	14144917	5
Caelo	Clotrimazol	14144918	12
Caelo	Clotrimazol	143337811	1
Caelo	Clotrimazol	14337801	14
Caelo	Clotrimazol	14337802	8
Caelo	Clotrimazol	14337807	12
Caelo	Clotrimazol	14337809	14
Caelo	Clotrimazol	14337811	4
Caelo	Clotrimazol	14337812	7
Caelo	Clotrimazol	14337813	8
Caelo	Clotrimazol	14337814	9
Caelo	Clotrimazol	14337815	10
Caelo	Clotrimazol	14337816	17
Caelo	Clotrimazol	14337817	17
Caelo	Clotrimazol	14337818	14
Caelo	Clotrimazol	14337819	8
Caelo	Clotrimazol	14337824	3
Caelo	Clotrimazol	14337824NP	1
Caelo	Clotrimazol	14337827	10
Caelo	Clotrimazol	14337828	13
Caelo	Clotrimazol	14337829	20
Caelo	Clotrimazol	14337830	3
Caelo	Clotrimazol	14337832	1
Caelo	Clotrimazol	14338712	1
Caelo	Clotrimazol	1437816	1
Caelo	Clotrimazol	14B05-B35	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	14B05-B36-291167	1
Caelo	Clotrimazol	14B05-B36-291168	1
Caelo	Clotrimazol	14c04-b30-291656	1
Caelo	Clotrimazol	14C04-B30-291656	2
Caelo	Clotrimazol	14c04-B31	1
Caelo	Clotrimazol	14C04-B31-294939	1
Caelo	Clotrimazol	14c04-b31-299954	2
Caelo	Clotrimazol	14C04B31-299954	1
Caelo	Clotrimazol	14C04-B31-299955	1
Caelo	Clotrimazol	14C04-B32-291657	1
Caelo	Clotrimazol	1510003-01	4
Caelo	Clotrimazol	15295603	1
Caelo	Clotrimazol	15395602	20
Caelo	Clotrimazol	15395603	10
Caelo	Clotrimazol	15395604	15
Caelo	Clotrimazol	15395605	15
Caelo	Clotrimazol	1539561	1
Caelo	Clotrimazol	15395610	7
Caelo	Clotrimazol	15395611	13
Caelo	Clotrimazol	15395613	8
Caelo	Clotrimazol	15395614	8
Caelo	Clotrimazol	15395615	8
Caelo	Clotrimazol	15395617	12
Caelo	Clotrimazol	15395618	20
Caelo	Clotrimazol	15395618I-81216/1	1
Caelo	Clotrimazol	15395623	2
Caelo	Clotrimazol	1539613	1
Caelo	Clotrimazol	153965604	1
Caelo	Clotrimazol	156546	1
Caelo	Clotrimazol	15G14-B05-311101	1
Caelo	Clotrimazol	15G14-B05-311103	2
Caelo	Clotrimazol	15G14-B05-316483	2
Caelo	Clotrimazol	15G14-B06-311054	1
Caelo	Clotrimazol	15G14-B06-311057	1
Caelo	Clotrimazol	16051913	1
Caelo	Clotrimazol	160614	1
Caelo	Clotrimazol	160704601	1
Caelo	Clotrimazol	1607046-01	7
Caelo	Clotrimazol	1607046-02	7
Caelo	Clotrimazol	16131901	1
Caelo	Clotrimazol	1623417	1
Caelo	Clotrimazol	16234501	8
Caelo	Clotrimazol	16234502	6
Caelo	Clotrimazol	16234503	19
Caelo	Clotrimazol	16234504	11
Caelo	Clotrimazol	16234505	30
Caelo	Clotrimazol	16234506	1
Caelo	Clotrimazol	16234509	11
Caelo	Clotrimazol	16234511	20
Caelo	Clotrimazol	16234512	19
Caelo	Clotrimazol	16234513	26
Caelo	Clotrimazol	162345135319	1
Caelo	Clotrimazol	16234515	1
Caelo	Clotrimazol	16234517	10
Caelo	Clotrimazol	16234520	25
Caelo	Clotrimazol	16234521	11
Caelo	Clotrimazol	16234522	23
Caelo	Clotrimazol	162345225555	1
Caelo	Clotrimazol	16234523	1
Caelo	Clotrimazol	16234525	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	1623455	1
Caelo	Clotrimazol	16B09-B06-3115007	1
Caelo	Clotrimazol	16B09B06311506	1
Caelo	Clotrimazol	16B09-B06-311785	1
Caelo	Clotrimazol	16B11-B04-320088	1
Caelo	Clotrimazol	16B11-B04-322393	1
Caelo	Clotrimazol	16B11-B04-325221	1
Caelo	Clotrimazol	16E20-B10	2
Caelo	Clotrimazol	16E20-B10-324555	1
Caelo	Clotrimazol	16J07-B02	1
Caelo	Clotrimazol	16J07-B02_330236	1
Caelo	Clotrimazol	16J07-B02-329385	4
Caelo	Clotrimazol	16J07-B02-329386	1
Caelo	Clotrimazol	16J07-B02-330216	2
Caelo	Clotrimazol	16J07-B02-335773	1
Caelo	Clotrimazol	16J07-B02-344817	1
Caelo	Clotrimazol	16J07-B02-344818	2
Caelo	Clotrimazol	17/25-B06-345048	1
Caelo	Clotrimazol	17011601	1
Caelo	Clotrimazol	1703028	1
Caelo	Clotrimazol	170302801	4
Caelo	Clotrimazol	1703028-01	12
Caelo	Clotrimazol	1703028-02	4
Caelo	Clotrimazol	170302803	1
Caelo	Clotrimazol	1703028-03	4
Caelo	Clotrimazol	1703028-0318147206	1
Caelo	Clotrimazol	17053186	1
Caelo	Clotrimazol	171113608	1
Caelo	Clotrimazol	17111601	15
Caelo	Clotrimazol	17111603	4
Caelo	Clotrimazol	17111604	8
Caelo	Clotrimazol	17111605	19
Caelo	Clotrimazol	17111606	30
Caelo	Clotrimazol	17111608	12
Caelo	Clotrimazol	1711161	1
Caelo	Clotrimazol	17111612	1
Caelo	Clotrimazol	17111613	27
Caelo	Clotrimazol	17111615	27
Caelo	Clotrimazol	17111616	35
Caelo	Clotrimazol	17111617	5
Caelo	Clotrimazol	1711603	2
Caelo	Clotrimazol	1711604	2
Caelo	Clotrimazol	1711605	1
Caelo	Clotrimazol	1711606	2
Caelo	Clotrimazol	1711613	2
Caelo	Clotrimazol	1711816	1
Caelo	Clotrimazol	17260204	1
Caelo	Clotrimazol	1736002001	1
Caelo	Clotrimazol	173600201	2
Caelo	Clotrimazol	17360023	1
Caelo	Clotrimazol	17360201	30
Caelo	Clotrimazol	17360202	36
Caelo	Clotrimazol	17360203	16
Caelo	Clotrimazol	17360204	29
Caelo	Clotrimazol	17A19-B04	1
Caelo	Clotrimazol	17A19-B04-332097	1
Caelo	Clotrimazol	17A19-B04-340476	1
Caelo	Clotrimazol	17J25-B06-345045	1
Caelo	Clotrimazol	17J25-B06-345048	1
Caelo	Clotrimazol	17J25-B06-347476	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	18016104	1
Caelo	Clotrimazol	1808028-01	8
Caelo	Clotrimazol	1808028-02	5
Caelo	Clotrimazol	18081408	1
Caelo	Clotrimazol	1814211	1
Caelo	Clotrimazol	18147101	47
Caelo	Clotrimazol	18147102	41
Caelo	Clotrimazol	18147103	24
Caelo	Clotrimazol	181471035763	1
Caelo	Clotrimazol	18147201	2
Caelo	Clotrimazol	18147202	2
Caelo	Clotrimazol	18147203	38
Caelo	Clotrimazol	18147206	1
Caelo	Clotrimazol	18147208	2
Caelo	Clotrimazol	18147210	56
Caelo	Clotrimazol	18147211	49
Caelo	Clotrimazol	18147212	13
Caelo	Clotrimazol	18147215	3
Caelo	Clotrimazol	18147216	7
Caelo	Clotrimazol	18147217	8
Caelo	Clotrimazol	1847103	1
Caelo	Clotrimazol	1882321	2
Caelo	Clotrimazol	1882404	1
Caelo	Clotrimazol	18A18-B05-347865	2
Caelo	Clotrimazol	18A18-B05-348429	1
Caelo	Clotrimazol	18A18-B05-349662	1
Caelo	Clotrimazol	18A18B05350778	1
Caelo	Clotrimazol	18A18-B05-350780	1
Caelo	Clotrimazol	18A18-B05-350781	1
Caelo	Clotrimazol	18A18-b05-352115	1
Caelo	Clotrimazol	18A18-B05-352115	1
Caelo	Clotrimazol	18A18-B05-353892	1
Caelo	Clotrimazol	18A18-B056-352115	1
Caelo	Clotrimazol	18G10-B06-352425	1
Caelo	Clotrimazol	18G10-B06-352427	2
Caelo	Clotrimazol	18g10-b06-358825	1
Caelo	Clotrimazol	190016207	1
Caelo	Clotrimazol	19015107	1
Caelo	Clotrimazol	190160106	1
Caelo	Clotrimazol	1901606	1
Caelo	Clotrimazol	19016103	19
Caelo	Clotrimazol	19016104	17
Caelo	Clotrimazol	19016105	29
Caelo	Clotrimazol	19016106	27
Caelo	Clotrimazol	19016107	27
Caelo	Clotrimazol	19016108	17
Caelo	Clotrimazol	19016115	1
Caelo	Clotrimazol	19016115P-191111-1	1
Caelo	Clotrimazol	19016116	29
Caelo	Clotrimazol	19016119	23
Caelo	Clotrimazol	190162001	2
Caelo	Clotrimazol	19016202	20
Caelo	Clotrimazol	19016203	22
Caelo	Clotrimazol	19016204	23
Caelo	Clotrimazol	19016205	12
Caelo	Clotrimazol	19016206	16
Caelo	Clotrimazol	19016207	1
Caelo	Clotrimazol	19016208	25
Caelo	Clotrimazol	19016210	2
Caelo	Clotrimazol	19016212	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	190200401	1
Caelo	Clotrimazol	1902004-01	4
Caelo	Clotrimazol	19052401	1
Caelo	Clotrimazol	1906106	1
Caelo	Clotrimazol	190652002	1
Caelo	Clotrimazol	1916202	1
Caelo	Clotrimazol	192004-03	1
Caelo	Clotrimazol	19B14-B01	1
Caelo	Clotrimazol	19B14-B01-359537	1
Caelo	Clotrimazol	19B14-B01-359539	2
Caelo	Clotrimazol	19J23-F06-367382	1
Caelo	Clotrimazol	200000	1
Caelo	Clotrimazol	200000000094008	1
Caelo	Clotrimazol	200000092005	1
Caelo	Clotrimazol	200000094003	1
Caelo	Clotrimazol	200000094004	2
Caelo	Clotrimazol	2000002005	1
Caelo	Clotrimazol	2000004002	1
Caelo	Clotrimazol	200000892006	1
Caelo	Clotrimazol	2000009	1
Caelo	Clotrimazol	20000092002	16
Caelo	Clotrimazol	20000092005	10
Caelo	Clotrimazol	20000092006	24
Caelo	Clotrimazol	20000092007	26
Caelo	Clotrimazol	2000009202	1
Caelo	Clotrimazol	2000009207	1
Caelo	Clotrimazol	20000094001	1
Caelo	Clotrimazol	20000094002	24
Caelo	Clotrimazol	20000094003	25
Caelo	Clotrimazol	200000940033	1
Caelo	Clotrimazol	20000094004	33
Caelo	Clotrimazol	20000094005	35
Caelo	Clotrimazol	20000094006	26
Caelo	Clotrimazol	2000009400601882404	1
Caelo	Clotrimazol	20000094007	1
Caelo	Clotrimazol	20000094008	20
Caelo	Clotrimazol	20000094009	1
Caelo	Clotrimazol	20000094012	1
Caelo	Clotrimazol	2000009404	2
Caelo	Clotrimazol	2000009408	1
Caelo	Clotrimazol	200003904005	1
Caelo	Clotrimazol	2000092002	1
Caelo	Clotrimazol	2000092006	1
Caelo	Clotrimazol	2000092007	1
Caelo	Clotrimazol	2000094003	1
Caelo	Clotrimazol	2000094004	1
Caelo	Clotrimazol	2000094005	1
Caelo	Clotrimazol	2000094008	3
Caelo	Clotrimazol	200009402	1
Caelo	Clotrimazol	20003904003	17
Caelo	Clotrimazol	20003904004	36
Caelo	Clotrimazol	20003904005	9
Caelo	Clotrimazol	20003904008	7
Caelo	Clotrimazol	2007033-01	4
Caelo	Clotrimazol	2007033-02	1
Caelo	Clotrimazol	2007033-03	1
Caelo	Clotrimazol	20111018	1
Caelo	Clotrimazol	20111115	1
Caelo	Clotrimazol	20160801	5
Caelo	Clotrimazol	2092	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	20H26F05373737	1
Caelo	Clotrimazol	21/24-B11-218638	1
Caelo	Clotrimazol	210000121002	1
Caelo	Clotrimazol	21000121002	43
Caelo	Clotrimazol	21000121003	27
Caelo	Clotrimazol	21000121004	47
Caelo	Clotrimazol	21000121005	2
Caelo	Clotrimazol	21000121006	24
Caelo	Clotrimazol	21000121008	13
Caelo	Clotrimazol	21000121009	28
Caelo	Clotrimazol	21000121010	29
Caelo	Clotrimazol	210001210101	1
Caelo	Clotrimazol	21000121013	15
Caelo	Clotrimazol	21000123006	17
Caelo	Clotrimazol	21000123008	23
Caelo	Clotrimazol	21000123010	9
Caelo	Clotrimazol	21000123011	17
Caelo	Clotrimazol	21000211006	1
Caelo	Clotrimazol	210004116005	1
Caelo	Clotrimazol	2100117013	1
Caelo	Clotrimazol	2100121009	1
Caelo	Clotrimazol	21004116001	12
Caelo	Clotrimazol	21004116003	7
Caelo	Clotrimazol	21004116005	9
Caelo	Clotrimazol	21004116006	3
Caelo	Clotrimazol	21004116007	2
Caelo	Clotrimazol	21004116008	1
Caelo	Clotrimazol	21004116013	2
Caelo	Clotrimazol	21004116014	3
Caelo	Clotrimazol	21004117001	12
Caelo	Clotrimazol	21004117003	3
Caelo	Clotrimazol	21004117004	9
Caelo	Clotrimazol	21004117005	10
Caelo	Clotrimazol	21004117007	19
Caelo	Clotrimazol	21004117011	2
Caelo	Clotrimazol	21004117013	1
Caelo	Clotrimazol	21004117016	9
Caelo	Clotrimazol	21004117017	5
Caelo	Clotrimazol	21004117018	5
Caelo	Clotrimazol	21004117019	1
Caelo	Clotrimazol	21004117022	2
Caelo	Clotrimazol	2100417005	1
Caelo	Clotrimazol	2103024-01	3
Caelo	Clotrimazol	210302402	2
Caelo	Clotrimazol	2103024-03	1
Caelo	Clotrimazol	21-24-B11-218638	1
Caelo	Clotrimazol	2217Q-01276	1
Caelo	Clotrimazol	23001596002	1
Caelo	Clotrimazol	26071305	1
Caelo	Clotrimazol	310316-5-461	1
Caelo	Clotrimazol	311111	1
Caelo	Clotrimazol	3335	1
Caelo	Clotrimazol	3456575	1
Caelo	Clotrimazol	412091-2-P	1
Caelo	Clotrimazol	415050-2-P	1
Caelo	Clotrimazol	418072-1-P	1
Caelo	Clotrimazol	5117E-01276	1
Caelo	Clotrimazol	54292100012113	1
Caelo	Clotrimazol	700135-0006	1
Caelo	Clotrimazol	8638446	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazol	94006	1
Caelo	Clotrimazol	94008	1
Caelo	Clotrimazol	AP1510003-01C	1
Caelo	Clotrimazol	Fagron	1
Caelo	Clotrimazol	HCZ14218	1
Caelo	Clotrimazol	HCZ20120	1
Caelo	Clotrimazol	P-21091821/18147203	1
Caelo	Clotrimazol	PC85	1
Caeolo/Gehe	Clotrimazol	16234521	1
Caesar & Lorenz GmbH	Clotrimazol	21004117016	1
Caesar & Loretz /Phönix	Clotrimazol	2000094004	1
Caesar & Loretz GmbH...	Clotrimazol	21004117007	1
Caesar & Loretz GmbH...	Clotrimazol	21000121009	1
Caesar & Loretz GmbH...	Clotrimazol	19016108	1
Caesar & Loretz GmbH...	Clotrimazol	20000092006	1
Caesar & Loretz GmbH...	Clotrimazol	200000094005	1
Caesar & Loretz GmbH...	Clotrimazol	21000123008	1
Caesar & Loretz GmbH...	Clotrimazol	19016202	2
Caesar & Loretz GmbH...	Clotrimazol	19016103	1
Caesar & Loretz GmbH...	Clotrimazol	21000121009	1
Caesar & Loretz GmbH Sana	Clotrimazol	21004117011	1
Caesar & Loretz GmbH...	Clotrimazol	18147203	1
Caesar & Loretz GmbH...	Clotrimazol	20000094003	3
Caesar & Loretz GmbH...	Clotrimazol	20003904004	1
Caesar & Loretz GmbH...	Clotrimazol	20000094003	1
Caesar & Loretz GmbH...	Clotrimazol	21000123006	1
Caesar & Loretz GmbH...	Clotrimazol	20000092006	1
Caesar & Loretz GmbH...	Clotrimazol	20000094002	1
Caesar & Loretz GmbH...	Clotrimazol	20000094003	1
Caesar & Loretz GmbH...	Clotrimazol	20003904003	1
Caesar & Loretz GmbH...	Clotrimazol	21000121004	1
Caesar & Loretz GmbH...	Clotrimazol	19016205	1
Caesar & Loretz GmbH/AEP	Clotrimazol	21000121009	1
Caesar & Loretz GmbH/AHD	Clotrimazol	18147211	1
Caesar & Loretz GmbH/AHD	Clotrimazol	21000121010	1
Caesar & Loretz GmbH/AHD	Clotrimazol	21004117004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121009	1
Caesar & Loretz GmbH...	Clotrimazol	19016105	1
Caesar & Loretz GmbH...	Clotrimazol	19016106	1
Caesar & Loretz GmbH...	Clotrimazol	20003904005	1
Caesar & Loretz GmbH...	Clotrimazol	21000123008	1
Caesar & Loretz GmbH/GEHE	Clotrimazol	18147211	1
Caesar & Loretz GmbH/Gehe	Clotrimazol	19016204	1
Caesar & Loretz GmbH/Gehe	Clotrimazol	20000092007	1
Caesar & Loretz GmbH/Gehe	Clotrimazol	20000094002	7
Caesar & Loretz GmbH/GEHE	Clotrimazol	20000094004	1
Caesar & Loretz GmbH/Gehe	Clotrimazol	21000121006	2
Caesar & Loretz GmbH/Gehe	Clotrimazol	21000123011	1
Caesar & Loretz GmbH/Gehe	Clotrimazol	21004117005	1
Caesar & Loretz GmbH...	Clotrimazol	20000092006	1
Caesar & Loretz GmbH...	Clotrimazol	21000121013	1
Caesar & Loretz GmbH...	Clotrimazol	21004116001	1
Caesar & Loretz GmbH...	Clotrimazol	19016105	1
Caesar & Loretz GmbH...	Clotrimazol	19016203	1
Caesar & Loretz GmbH...	Clotrimazol	20000094004	1
Caesar & Loretz GmbH...	Clotrimazol	20003904004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121003	1
Caesar & Loretz GmbH...	Clotrimazol	19016206	1
Caesar & Loretz GmbH...	Clotrimazol	20003904003	1
Caesar & Loretz GmbH...	Clotrimazol	21000121010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Clotrimazol	21000123011	1
Caesar & Loretz GmbH/K	Clotrimazol	20003904004	1
Caesar & Loretz GmbH...	Clotrimazol	20000094004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121006	1
Caesar & Loretz GmbH...	Clotrimazol	18147102	1
Caesar & Loretz GmbH...	Clotrimazol	20000094002	1
Caesar & Loretz GmbH...	Clotrimazol	20000094005	1
Caesar & Loretz GmbH...	Clotrimazol	20000094008	1
Caesar & Loretz GmbH...	Clotrimazol	21000123006	1
Caesar & Loretz GmbH...	Clotrimazol	21000121006	1
Caesar & Loretz GmbH/Pho	Clotrimazol	21000121004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121002	1
Caesar & Loretz GmbH...	Clotrimazol	21000123008	1
Caesar & Loretz GmbH...	Clotrimazol	21004116001	1
Caesar & Loretz GmbH...	Clotrimazol	21004116003	1
Caesar & Loretz GmbH...	Clotrimazol	21004117022	1
Caesar & Loretz GmbH...	Clotrimazol	20000094004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121009	1
Caesar & Loretz GmbH...	Clotrimazol	21000121013	1
Caesar & Loretz GmbH...	Clotrimazol	21000123006	2
Caesar & Loretz GmbH...	Clotrimazol	21000123010	2
Caesar & Loretz GmbH...	Clotrimazol	20003904005	1
Caesar & Loretz GmbH...	Clotrimazol	21000121009	1
Caesar & Loretz GmbH...	Clotrimazol	19016119	2
Caesar & Loretz GmbH...	Clotrimazol	19016203	1
Caesar & Loretz GmbH...	Clotrimazol	19016204	1
Caesar & Loretz GmbH...	Clotrimazol	20000092005	1
Caesar & Loretz GmbH...	Clotrimazol	20000092007	1
Caesar & Loretz GmbH...	Clotrimazol	20000094004	1
Caesar & Loretz GmbH...	Clotrimazol	20000094006	2
Caesar & Loretz GmbH...	Clotrimazol	20003904004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121002	2
Caesar & Loretz GmbH...	Clotrimazol	21000121003	2
Caesar & Loretz GmbH...	Clotrimazol	21000121004	1
Caesar & Loretz GmbH...	Clotrimazol	21000121008	1
Caesar & Loretz GmbH...	Clotrimazol	21000121009	2
Caesar & Loretz GmbH...	Clotrimazol	21000121010	1
Caesar & Loretz GmbH...	Clotrimazol	AP210225-03	1
Caesar & Loretz GmbH...	Clotrimazol	AP210622-01	1
Caesar & Loretz GmbH	Clotrimazol	16J07B02344817	1
Caesar & Loretz GmbH	Clotrimazol	17111604	1
Caesar & Loretz GmbH	Clotrimazol	17360204	3
Caesar & Loretz GmbH	Clotrimazol	17A19-B04	1
Caesar & Loretz GmbH	Clotrimazol	18147103	1
Caesar & Loretz GmbH	Clotrimazol	18147203	1
Caesar & Loretz GmbH	Clotrimazol	18147210	13
Caesar & Loretz GmbH	Clotrimazol	18147211	5
Caesar & Loretz GmbH	Clotrimazol	18147212	2
Caesar & Loretz GmbH	Clotrimazol	18147216	2
Caesar & Loretz GmbH	Clotrimazol	18147217	2
Caesar & Loretz GmbH	Clotrimazol	19016103	1
Caesar & Loretz GmbH	Clotrimazol	19016104	2
Caesar & Loretz GmbH	Clotrimazol	19016105	9
Caesar & Loretz GmbH	Clotrimazol	19016106	6
Caesar & Loretz GmbH	Clotrimazol	19016107	5
Caesar & Loretz GmbH	Clotrimazol	19016108	5
Caesar & Loretz GmbH	Clotrimazol	19016116	10
Caesar & Loretz GmbH	Clotrimazol	19016119	11
Caesar & Loretz GmbH	Clotrimazol	190162001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Clotrimazol	19016202	11
Caesar & Loretz GmbH	Clotrimazol	19016203	5
Caesar & Loretz GmbH	Clotrimazol	19016204	5
Caesar & Loretz GmbH	Clotrimazol	19016205	4
Caesar & Loretz GmbH	Clotrimazol	19016206	1
Caesar & Loretz GmbH	Clotrimazol	19016208	9
Caesar & Loretz GmbH	Clotrimazol	1902004-02	1
Caesar & Loretz GmbH	Clotrimazol	19076708	3
Caesar & Loretz GmbH	Clotrimazol	20000092002	7
Caesar & Loretz GmbH	Clotrimazol	20000092005	3
Caesar & Loretz GmbH	Clotrimazol	20000092006	14
Caesar & Loretz GmbH	Clotrimazol	20000092007	8
Caesar & Loretz GmbH	Clotrimazol	20000094002	2
Caesar & Loretz GmbH	Clotrimazol	20000094003	1
Caesar & Loretz GmbH	Clotrimazol	20000094004	8
Caesar & Loretz GmbH	Clotrimazol	20000094005	13
Caesar & Loretz GmbH	Clotrimazol	20000094006	13
Caesar & Loretz GmbH	Clotrimazol	20000094007	1
Caesar & Loretz GmbH	Clotrimazol	20000094008	9
Caesar & Loretz GmbH	Clotrimazol	20000094012	1
Caesar & Loretz GmbH	Clotrimazol	2000094004	2
Caesar & Loretz GmbH	Clotrimazol	2000094006	1
Caesar & Loretz GmbH	Clotrimazol	20003904002	2
Caesar & Loretz GmbH	Clotrimazol	20003904003	1
Caesar & Loretz GmbH	Clotrimazol	20003904004	13
Caesar & Loretz GmbH	Clotrimazol	20003904005	10
Caesar & Loretz GmbH	Clotrimazol	20003904008	2
Caesar & Loretz GmbH	Clotrimazol	21000121002	8
Caesar & Loretz GmbH	Clotrimazol	21000121003	11
Caesar & Loretz GmbH	Clotrimazol	21000121004	15
Caesar & Loretz GmbH	Clotrimazol	21000121005	1
Caesar & Loretz GmbH	Clotrimazol	21000121006	22
Caesar & Loretz GmbH	Clotrimazol	21000121008	2
Caesar & Loretz GmbH	Clotrimazol	21000121009	12
CAESAR & LORETZ GMBH	Clotrimazol	21000121009	1
Caesar & Loretz GmbH	Clotrimazol	21000121010	12
Caesar & Loretz GmbH	Clotrimazol	21000121013	9
Caesar & Loretz GmbH	Clotrimazol	21000123003	1
Caesar & Loretz GmbH	Clotrimazol	21000123006	15
Caesar & Loretz GmbH	Clotrimazol	21000123008	7
Caesar & Loretz GmbH	Clotrimazol	21000123010	2
Caesar & Loretz GmbH	Clotrimazol	21000123011	7
Caesar & Loretz GmbH	Clotrimazol	21004116001	13
Caesar & Loretz GmbH	Clotrimazol	21004116003	1
Caesar & Loretz GmbH	Clotrimazol	21004116005	2
Caesar & Loretz GmbH	Clotrimazol	21004116007	4
Caesar & Loretz GmbH	Clotrimazol	21004116014	5
Caesar & Loretz GmbH	Clotrimazol	21004117001	1
Caesar & Loretz GmbH	Clotrimazol	21004117003	1
Caesar & Loretz GmbH	Clotrimazol	21004117004	8
Caesar & Loretz GmbH	Clotrimazol	21004117005	10
Caesar & Loretz GmbH	Clotrimazol	21004117007	13
Caesar & Loretz GmbH	Clotrimazol	21004117011	3
Caesar & Loretz GmbH	Clotrimazol	21004117013	1
Caesar & Loretz GmbH	Clotrimazol	21004117016	2
Caesar & Loretz GmbH	Clotrimazol	21004117017	3
Caesar & Loretz GmbH	Clotrimazol	21004117018	2
Caesar & Loretz GmbH	Clotrimazol	21004117022	2
Caesar & Loretz GmbH	Clotrimazol	21I24-B11-213292	1
Caesar & Loretz GmbH...	Clotrimazol	20000092006	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Clotrimazol	20000094006	1
Caesar & Loretz Hild...	Clotrimazol	20003904003	1
Caesar & Loretz Hilden	Clotrimazol	18147211	1
Caesar & Loretz Hilden	Clotrimazol	19016204	1
Caesar & Loretz Hilden	Clotrimazol	20000094004	1
Caesar & Loretz/Geil...	Clotrimazol	18147203	1
Caesar & Loretz/Geil...	Clotrimazol	20000092005	1
Caesar & Loretz/Geil...	Clotrimazol	21000121002	2
Caesar & Loretz/Noweda	Clotrimazol	20000094002	1
Caesar & Loretz/Noweda	Clotrimazol	20000094005	1
Caesar & Loretz/Sanacorp	Clotrimazol	18147210	1
Caesar & Loretz	Clotrimazol	16234504	1
Caesar & Loretz	Clotrimazol	H20160502	1
Caesar u Loretz	Clotrimazol	15395613	1
Caesar u Loretz	Clotrimazol	16234501	1
Caesar&Lorenz / Gehe	Clotrimazol	19016199	1
Caesar&Lorenz	Clotrimazol	21000121002	1
Caesar&Loretz GmbH,1...	Clotrimazol	16234509	1
caesar&loretz GmbH,P...	Clotrimazol	15395614	1
Caesar&Loretz GmbH/ ...	Clotrimazol	16234522	1
Caesar&Loretz GmbH/Anzag	Clotrimazol	13184111	1
Caesar&Loretz GmbH/Anzag	Clotrimazol	14337807	1
Caesar&Loretz GmbH	Clotrimazol	14337814	1
Caesar&loretz,Phoenix	Clotrimazol	14144912	1
Caesar&LoretzGmbH, P...	Clotrimazol	18147212	1
Caesar/Gehe	Clotrimazol	20000092006	2
Caesar/Lorenz	Clotrimazol	12320814	1
Caesar/Lorenz	Clotrimazol	13224201	3
Caleo	Clotrimazol	15395610	1
CALO	Clotrimazol	17360204	1
Cealo/ Anzag	Clotrimazol	1703028-01	2
Cealo/GEHE	Clotrimazol	18147101	2
Cealo/Phoenix	Clotrimazol	19016106	1
Cealo/Sanacorp	Clotrimazol	1902004-03	1
Cealo	Clotrimazol	15395610	1
Cealo	Clotrimazol	17111612	1
Cealo	Clotrimazol	18147210	1
Delta	Clotrimazol	1607046-01	1
Dr. Wolff	Clotrimazol	1409027-04	2
E Plus	Clotrimazol	1703028-02	1
E Plus	Clotrimazol	1808028-01	2
EuRho / Phoenix	Clotrimazol	1703028-01	1
EuRho / Phoenix	Clotrimazol	2103024-02	4
EuRho / Phönix	Clotrimazol	2103024-01	1
EuRho /Gehe	Clotrimazol	1409027-02	1
EuRho AHC	Clotrimazol	1306036-01	1
EuRho Noweda	Clotrimazol	2007033-02	1
EuRho Noweda	Clotrimazol	2103024-01	1
EuRho/ Anzag	Clotrimazol	220629(2103024-01)	1
EuRho/ Fiebig	Clotrimazol	2007033-01	1
EuRho/ Phoenix	Clotrimazol	160704602	1
EuRho/ Phönix	Clotrimazol	1703028-02	1
EuRho/Gehe	Clotrimazol	2007033-01	1
EuRho/Gehe	Clotrimazol	2103024-01	1
EuRho/Kehr	Clotrimazol	1703028-02	1
EuRho/Noweda	Clotrimazol	2103024-02	1
EuRho/Phoenix	Clotrimazol	1210039-02	1
EuRho/Phoenix	Clotrimazol	1409027-01	1
EuRho/Phoenix	Clotrimazol	2007033-01	2
EuRho/Phoenix	Clotrimazol	2007033-03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Phönix	Clotrimazol	1210039-2	1
EuRho/Phönix	Clotrimazol	1808028-01	1
Eurho/Phönix	Clotrimazol	200703302	1
EuRho/Sanacorp	Clotrimazol	16234522	1
EuRho	Clotrimazol	1108053-02	1
EuRho	Clotrimazol	1203040-02	2
EuRho	Clotrimazol	1203040-03	1
EuRho	Clotrimazol	1210039-02	2
EuRho	Clotrimazol	1306036-01	2
eurho	Clotrimazol	1309034-01	1
eurho	Clotrimazol	1309034-02	2
EuRho	Clotrimazol	1309034-02	1
EuRho	Clotrimazol	1409027-01	2
EuRho	Clotrimazol	1703028-01	2
Eurho	Clotrimazol	1703028-02	2
EuRho	Clotrimazol	18080028-01	1
EuRho	Clotrimazol	1808028-01	1
EuRho	Clotrimazol	1902004-01	5
EuRho	Clotrimazol	1902004-02	3
EuRho	Clotrimazol	1902204-01	1
EuRho	Clotrimazol	2007033-01	2
EuRho	Clotrimazol	2007033-02	1
EuRho	Clotrimazol	2103024-01	2
EuRhoNoweda	Clotrimazol	2103024-01	1
EuRhoPh/Ph	Clotrimazol	1902004-02	2
EuRhoPh/Ph	Clotrimazol	2007033-0130	1
Euro /BAUMANN	Clotrimazol	2007033-01	1
Euro Gehe	Clotrimazol	1808028-01	1
Euro OCT Pharma/ Sanacorp	Clotrimazol	1409027-04	1
Euro OT/Gehe	Clotrimazol	1409027-03	2
Euro OTC	Clotrimazol		6
Euro OTC	Clotrimazol	1008028	1
Euro OTC	Clotrimazol	1105014-01	1
Euro OTC	Clotrimazol	110501402	1
Euro OTC	Clotrimazol	1105014-02	1
Euro OTC	Clotrimazol	1108053-01	1
Euro OTC	Clotrimazol	1108053-02	2
Euro OTC	Clotrimazol	11808028-01	1
Euro OTC	Clotrimazol	1202004-03	1
Euro OTC	Clotrimazol	1203040	1
Euro OTC	Clotrimazol	1203040-01	1
Euro OTC	Clotrimazol	120304002	1
Euro OTC	Clotrimazol	1203040-02	8
Euro OTC	Clotrimazol	1203040-03	9
Euro OTC	Clotrimazol	12082013C	1
Euro OTC	Clotrimazol	1209211276	1
Euro OTC	Clotrimazol	121003901	3
Euro OTC	Clotrimazol	1210039-01	24
Euro OTC	Clotrimazol	1210039-02	22
Euro OTC	Clotrimazol	1306036	1
Euro OTC	Clotrimazol	130603601	3
Euro OTC	Clotrimazol	1306036-01	39
Euro OTC	Clotrimazol	1306306-01	1
Euro OTC	Clotrimazol	130636-01	2
Euro OTC	Clotrimazol	1309034	1
Euro OTC	Clotrimazol	130903401	5
Euro OTC	Clotrimazol	1309034-01	21
Euro OTC	Clotrimazol	130903402	1
Euro OTC	Clotrimazol	1309034-02	21
Euro OTC	Clotrimazol	1309054-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clotrimazol	1314Q1276	1
Euro OTC	Clotrimazol	13418014	1
Euro OTC	Clotrimazol	1409027	6
Euro OTC	Clotrimazol	1409027_03	1
Euro OTC	Clotrimazol	140902701	1
Euro OTC	Clotrimazol	1409027-01	29
Euro OTC	Clotrimazol	140902702	3
Euro OTC	Clotrimazol	1409027-02	44
Euro OTC	Clotrimazol	1409027-02Mg10g	1
Euro OTC	Clotrimazol	1409027-03	22
Euro OTC	Clotrimazol	1409027-04	30
Euro OTC	Clotrimazol	140927-01	1
Euro OTC	Clotrimazol	140927-02	1
Euro OTC	Clotrimazol	14144914	1
Euro OTC	Clotrimazol	14C04-B31-291660	1
Euro OTC	Clotrimazol	150003-01	1
Euro OTC	Clotrimazol	150003-02	1
Euro OTC	Clotrimazol	15010003-01	1
Euro OTC	Clotrimazol	15042014C	1
Euro OTC	Clotrimazol	15072014A	1
Euro OTC	Clotrimazol	151000	1
Euro OTC	Clotrimazol	151000-01	1
Euro OTC	Clotrimazol	1510003_01	1
Euro OTC	Clotrimazol	151000301	1
Euro OTC	Clotrimazol	1510003-01	57
Euro OTC	Clotrimazol	1510003-02	24
Euro OTC	Clotrimazol	151003-01	1
Euro OTC	Clotrimazol	1605003C	1
Euro OTC	Clotrimazol	1607045-01	1
Euro OTC	Clotrimazol	1607046	1
Euro OTC	Clotrimazol	1607046-0	1
Euro OTC	Clotrimazol	160704601	5
Euro OTC	Clotrimazol	1607046-01	71
Euro OTC	Clotrimazol	160704602	2
Euro OTC	Clotrimazol	1607046-02	40
Euro OTC	Clotrimazol	1607064-01	1
Euro OTC	Clotrimazol	16074046-01	1
Euro OTC	Clotrimazol	160802801	1
Euro OTC	Clotrimazol	1609046-01	1
Euro OTC	Clotrimazol	16234504	1
Euro OTC	Clotrimazol	16234505	1
Euro OTC	Clotrimazol	16234511	1
Euro OTC	Clotrimazol	16B11-B04-320088	1
Euro OTC	Clotrimazol	16J07-B02-341842	1
Euro OTC	Clotrimazol	170028-01	1
Euro OTC	Clotrimazol	1703025-03	1
Euro OTC	Clotrimazol	1703028	5
Euro OTC	Clotrimazol	1703028/03	1
Euro OTC	Clotrimazol	170302801	7
Euro OTC	Clotrimazol	1703028-01	119
Euro OTC	Clotrimazol	170302801-01	1
Euro OTC	Clotrimazol	170302802	1
Euro OTC	Clotrimazol	1703028-02	73
Euro OTC	Clotrimazol	1703028-02	1
Euro OTC	Clotrimazol	170302803	2
Euro OTC	Clotrimazol	1703028-03	62
Euro OTC	Clotrimazol	17053183	1
Euro OTC	Clotrimazol	170615C/1703028-01	1
Euro OTC	Clotrimazol	17111606	1
Euro OTC	Clotrimazol	17360201	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clotrimazol	17A021	1
Euro OTC	Clotrimazol	17J25B06347476	1
Euro OTC	Clotrimazol	180002801	1
Euro OTC	Clotrimazol	180028-01	1
Euro OTC	Clotrimazol	1808018-01	1
Euro OTC	Clotrimazol	1808025-01	1
Euro OTC	Clotrimazol	1808028	4
Euro OTC	Clotrimazol	1808028_01	1
Euro OTC	Clotrimazol	1808028_02	1
Euro OTC	Clotrimazol	180802801	5
Euro OTC	Clotrimazol	1808028-01	129
Euro OTC	Clotrimazol	180802802	1
Euro OTC	Clotrimazol	1808028-02	79
Euro OTC	Clotrimazol	1808828-01	1
Euro OTC	Clotrimazol	18147211	1
Euro OTC	Clotrimazol	1828028-01	1
Euro OTC	Clotrimazol	19016108	1
Euro OTC	Clotrimazol	1902001-01	1
Euro OTC	Clotrimazol	1902004	2
Euro OTC	Clotrimazol	1902004_01	1
Euro OTC	Clotrimazol	190200401	7
Euro OTC	Clotrimazol	1902004-01	172
Euro OTC	Clotrimazol	1902004-01HZC14218	1
Euro OTC	Clotrimazol	190200402	1
Euro OTC	Clotrimazol	1902004-02	82
Euro OTC	Clotrimazol	190200403	2
Euro OTC	Clotrimazol	1902004-03	58
Euro OTC	Clotrimazol	190202004-02	1
Euro OTC	Clotrimazol	190204-01	2
Euro OTC	Clotrimazol	190204-03	1
Euro OTC	Clotrimazol	19022004-01	1
Euro OTC	Clotrimazol	19024004-01	1
Euro OTC	Clotrimazol	1904004-02	1
Euro OTC	Clotrimazol	192004-01	2
Euro OTC	Clotrimazol	20007033-01	1
Euro OTC	Clotrimazol	2007003-01	1
Euro OTC	Clotrimazol	200703-02	1
Euro OTC	Clotrimazol	2007033	1
Euro OTC	Clotrimazol	2007033_01	1
Euro OTC	Clotrimazol	200703301	5
Euro OTC	Clotrimazol	2007033-01	135
Euro OTC	Clotrimazol	2007033-02	70
Euro OTC	Clotrimazol	2007033-03	10
Euro OTC	Clotrimazol	2007033-1	1
Euro OTC	Clotrimazol	200733-02	1
Euro OTC	Clotrimazol	20130512	1
Euro OTC	Clotrimazol	20160801	5
Euro OTC	Clotrimazol	203024-02	1
Euro OTC	Clotrimazol	206718	1
Euro OTC	Clotrimazol	2103024	2
Euro OTC	Clotrimazol	2103024_02	1
Euro OTC	Clotrimazol	210302401	2
Euro OTC	Clotrimazol	2103024-01	85
Euro OTC	Clotrimazol	210302402	2
Euro OTC	Clotrimazol	2103024-02	46
Euro OTC	Clotrimazol	2103024-03	3
Euro OTC	Clotrimazol	2103024-04	1
Euro OTC	Clotrimazol	2103025-01	1
Euro OTC	Clotrimazol	21052015B	1
Euro OTC	Clotrimazol	21122013A	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clotrimazol	213024-02	1
Euro OTC	Clotrimazol	220425D	1
Euro OTC	Clotrimazol	22091806	1
Euro OTC	Clotrimazol	22122014B	1
Euro OTC	Clotrimazol	2214A-01276	1
Euro OTC	Clotrimazol	230105501	3
Euro OTC	Clotrimazol	2301055-01	3
Euro OTC	Clotrimazol	23121408	1
Euro OTC	Clotrimazol	2313M01276	1
Euro OTC	Clotrimazol	2785	1
Euro OTC	Clotrimazol	2881	1
Euro OTC	Clotrimazol	30011402	1
Euro OTC	Clotrimazol	30062002	1
Euro OTC	Clotrimazol	3118A-01276	1
Euro OTC	Clotrimazol	3912E-01276	1
Euro OTC	Clotrimazol	40714/05	1
Euro OTC	Clotrimazol	41(1808028-01)	1
Euro OTC	Clotrimazol	4216M01276	1
Euro OTC	Clotrimazol	4216M-01276	2
Euro OTC	Clotrimazol	6051501	1
Euro OTC	Clotrimazol	700135	2
Euro OTC	Clotrimazol	H20160502	1
Euro OTC	Clotrimazol	HCZ00720	1
Euro OTC	Clotrimazol	HCZ06718	3
Euro OTC	Clotrimazol	HCZ07720	3
Euro OTC	Clotrimazol	HCZ14218	4
Euro OTC	Clotrimazol	HCZ20120	2
euro//Noweda	Clotrimazol	1808028-01	1
EUro/AHD	Clotrimazol	1210039-01	2
Euro/Gehe	Clotrimazol	1607046-02	1
Euro/Gehe	Clotrimazol	1703028-03	1
Euro/Gehe	Clotrimazol	18A18-B05-350778	1
Euro/Noweda	Clotrimazol	1510003-02	1
EURO/Noweda	Clotrimazol	190200401	1
Euro/Phönix	Clotrimazol	1510003-02	1
Euro/Phönix	Clotrimazol	1808028-01	1
Euro/Phönix	Clotrimazol	1902004-01	2
Euro/Sanacorp	Clotrimazol	1703028-02	1
Euro/Sanacorp	Clotrimazol	1808028-01	2
Euro	Clotrimazol	1510003-01	2
Euro	Clotrimazol	160704601	1
EuRoh/ Gehe	Clotrimazol	1808028-01	2
Euroo / Phönix	Clotrimazol	1409027-02	3
Europ Ots Pharma	Clotrimazol	13184105	1
Europharm/Otto	Clotrimazol	1203040-01	1
Europharm/Otto	Clotrimazol	1203040-02	1
europharma	Clotrimazol	1306036-01	1
EuroTOC / Noweda	Clotrimazol	1409027-03	1
Faggron	Clotrimazol	21/24-B11-213293	2
Fagron	Clotrimazol		5
Fagron	Clotrimazol	10G10B06-352427	1
Fagron	Clotrimazol	11A05-N14	2
Fagron	Clotrimazol	11E17-N10	2
Fagron	Clotrimazol	11F30-N14	2
Fagron	Clotrimazol	11G15-N10	1
Fagron	Clotrimazol	11K21-N19	1
Fagron	Clotrimazol	11L12-N10	5
Fagron	Clotrimazol	12/21-N01	5
Fagron	Clotrimazol	12/21-N04	3
Fagron	Clotrimazol	1210039-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazol	1221n04	1
Fagron	Clotrimazol	1221N04	1
Fagron	Clotrimazol	12721-N01	1
Fagron	Clotrimazol	12a05-n10	1
Fagron	Clotrimazol	12A05-N10	2
Fagron	Clotrimazol	12B27-N05	3
Fagron	Clotrimazol	12e02-N12	1
Fagron	Clotrimazol	12E02-N12	9
Fagron	Clotrimazol	12E30-N02	1
Fagron	Clotrimazol	12E30-N07	11
Fagron	Clotrimazol	12F02-N12	1
Fagron	Clotrimazol	12I16-N04	1
Fagron	Clotrimazol	12I21-N01	7
Fagron	Clotrimazol	12I21N04	1
Fagron	Clotrimazol	12I21-N04	7
Fagron	Clotrimazol	12K15-N01	1
Fagron	Clotrimazol	12l21-N04	2
Fagron	Clotrimazol	1309034-01	3
Fagron	Clotrimazol	13224201	1
Fagron	Clotrimazol	13C25-N10	9
Fagron	Clotrimazol	1409027-02	1
Fagron	Clotrimazol	14223201	1
Fagron	Clotrimazol	14337801	1
Fagron	Clotrimazol	14337818	1
Fagron	Clotrimazol	14337827	1
Fagron	Clotrimazol	14B05-B35	2
Fagron	Clotrimazol	14B05-B35-293542	3
Fagron	Clotrimazol	14B05-B35-293543	2
Fagron	Clotrimazol	14b05-b35-293544	1
Fagron	Clotrimazol	14B05-B35-293544	6
Fagron	Clotrimazol	14B05-B35-294932	1
Fagron	Clotrimazol	14b05-b35-294935	1
Fagron	Clotrimazol	14B05B35294935	1
Fagron	Clotrimazol	14B05-B35-294935	4
Fagron	Clotrimazol	14b05-b35-299941	1
Fagron	Clotrimazol	14B05-B35-299941	2
Fagron	Clotrimazol	14B05-B35-299944	3
Fagron	Clotrimazol	14B05-B36	7
Fagron	Clotrimazol	14B05B36291165	1
Fagron	Clotrimazol	14B05-B36-291165	2
Fagron	Clotrimazol	14b05b36291166	1
Fagron	Clotrimazol	14b05-b36-291166	1
Fagron	Clotrimazol	14B05-B36-291166	3
Fagron	Clotrimazol	14b05-B36-291167	1
Fagron	Clotrimazol	14B05B36291167	1
Fagron	Clotrimazol	14B05-B36-291167	5
Fagron	Clotrimazol	14B05-B36-291168	2
Fagron	Clotrimazol	14B05-B36-2991166	1
Fagron	Clotrimazol	14B06-B06	1
Fagron	Clotrimazol	14B06-B06-299942	1
Fagron	Clotrimazol	14B06-B06-299943	6
Fagron	Clotrimazol	14C04-B30	1
Fagron	Clotrimazol	14C04-B30-291656	10
Fagron	Clotrimazol	14C04-B30-291661	3
Fagron	Clotrimazol	14C04B31	1
Fagron	Clotrimazol	14C04-B31	8
Fagron	Clotrimazol	14C04-B312-299959	1
Fagron	Clotrimazol	14C04-B31-291660	4
Fagron	Clotrimazol	14C04-B31-294939	6
Fagron	Clotrimazol	14C04-B31-294940	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazol	14C04-B31-294951	1
Fagron	Clotrimazol	14C04-B31-294952	1
Fagron	Clotrimazol	14C04-B31-299954	7
Fagron	Clotrimazol	14C04-B31-299955	1
Fagron	Clotrimazol	14C04-B31-299959	2
Fagron	Clotrimazol	14C04-B31-299960	7
Fagron	Clotrimazol	14C04B32291657	1
Fagron	Clotrimazol	14C04-B32-291657	1
Fagron	Clotrimazol	14E26-B02	1
Fagron	Clotrimazol	1510003-01	1
Fagron	Clotrimazol	15G14-B05	4
Fagron	Clotrimazol	15G14-B05-311100	12
Fagron	Clotrimazol	15G14-B05-311101	1
Fagron	Clotrimazol	15G14-B05-311102	4
Fagron	Clotrimazol	15G14-B05-311103	13
Fagron	Clotrimazol	15G14-B05-316483	1
Fagron	Clotrimazol	15G14-B06	1
Fagron	Clotrimazol	15G14-B06-211057	1
Fagron	Clotrimazol	15G14-B06-31105	1
Fagron	Clotrimazol	15g14-b06-311054	1
Fagron	Clotrimazol	15G14B06311054	1
Fagron	Clotrimazol	15G14B06-311054	1
Fagron	Clotrimazol	15G14-B06-311054	4
Fagron	Clotrimazol	15G14-B06-311055	2
Fagron	Clotrimazol	15G14-B06-311056	2
Fagron	Clotrimazol	15G14-Bo5-311101	1
Fagron	Clotrimazol	160704602	1
Fagron	Clotrimazol	16234521	2
Fagron	Clotrimazol	16607-B02-333606	1
Fagron	Clotrimazol	16B09-B06	1
Fagron	Clotrimazol	16B09-B06-311506	4
Fagron	Clotrimazol	16B09-B06-311507	5
Fagron	Clotrimazol	16B09-B06-311785	2
Fagron	Clotrimazol	16B11B04	1
Fagron	Clotrimazol	16B11-B04	1
Fagron	Clotrimazol	16B11-B04-320088	6
Fagron	Clotrimazol	16B11-B04-322393	2
Fagron	Clotrimazol	16B11-B04-327611	6
Fagron	Clotrimazol	16BB11B04327611	1
Fagron	Clotrimazol	16E20-B10-317566	2
Fagron	Clotrimazol	16E20-B10-321597	2
Fagron	Clotrimazol	16E20-B10-321598	11
Fagron	Clotrimazol	16E20-B10-32197	1
Fagron	Clotrimazol	16E20-B10-324555	5
Fagron	Clotrimazol	16E20-B10-326010	3
Fagron	Clotrimazol	16E20-B10-327349	7
Fagron	Clotrimazol	16J07_B02	1
Fagron	Clotrimazol	16J07-B02	2
Fagron	Clotrimazol	16J07-B02-329385	4
Fagron	Clotrimazol	16J07-B02-329386	3
Fagron	Clotrimazol	16J07-B02-330216	7
Fagron	Clotrimazol	16J07-B02-330236	2
Fagron	Clotrimazol	16J07-B02-3335773	1
Fagron	Clotrimazol	16J07-B02-333606	3
Fagron	Clotrimazol	16J07-B02-335773	2
Fagron	Clotrimazol	16J07-B02-337573	3
Fagron	Clotrimazol	16J07-B02-338283	8
Fagron	Clotrimazol	16J07-B02-340511	2
Fagron	Clotrimazol	16j07-b02-340513	2
Fagron	Clotrimazol	16J07-B02-340513	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazol	16J07-B02-340513-201	1
Fagron	Clotrimazol	16J07B02341842	2
Fagron	Clotrimazol	16J07-B02-341842	1
Fagron	Clotrimazol	16J07-B02-344816	2
Fagron	Clotrimazol	16J07-B02-344817	4
Fagron	Clotrimazol	16J07-B02-344818	8
Fagron	Clotrimazol	16J07B02347864	1
Fagron	Clotrimazol	16J07-B02-347864	4
Fagron	Clotrimazol	16J23-F06-365713	1
Fagron	Clotrimazol	1703028-01	1
Fagron	Clotrimazol	1703028-03	1
Fagron	Clotrimazol	17111613	1
Fagron	Clotrimazol	17360201	1
Fagron	Clotrimazol	17A19-804-38560	2
Fagron	Clotrimazol	17A19-B04_332114	1
Fagron	Clotrimazol	17A19-B04-332097	2
Fagron	Clotrimazol	17A19-B04332114	1
Fagron	Clotrimazol	17A19-B04-332114	2
Fagron	Clotrimazol	17A19-B04-334768	4
Fagron	Clotrimazol	17A19-B04-336568	1
Fagron	Clotrimazol	17A19-B04-336581	1
Fagron	Clotrimazol	17A19-B04-338560	4
Fagron	Clotrimazol	17A19-B04-338577	4
Fagron	Clotrimazol	17A19-B04-340476	1
Fagron	Clotrimazol	17A19-B04-336568	1
Fagron	Clotrimazol	17A19-SB04-332097	1
Fagron	Clotrimazol	17J25-B06	3
Fagron	Clotrimazol	17J25-B06-345044	5
Fagron	Clotrimazol	17J25-B06-345045	2
Fagron	Clotrimazol	17J25-B06-345048	2
Fagron	Clotrimazol	17J25-B06-345049	1
Fagron	Clotrimazol	17J25-B06-345406	1
Fagron	Clotrimazol	17J25-B06-345407	3
Fagron	Clotrimazol	17J25-B06-347476	5
Fagron	Clotrimazol	17J25-B06-349130	2
Fagron	Clotrimazol	17j25-B06-349161	1
Fagron	Clotrimazol	17J25-B06-349161	6
Fagron	Clotrimazol	17J25-Bo6-345045	1
Fagron	Clotrimazol	17J25-BO6-349161	1
Fagron	Clotrimazol	18147101	1
Fagron	Clotrimazol	18147102	1
Fagron	Clotrimazol	18147217	1
Fagron	Clotrimazol	18610_B06	1
Fagron	Clotrimazol	18A18B05	1
Fagron	Clotrimazol	18A18-B05	1
Fagron	Clotrimazol	18A18-B05-344819	1
Fagron	Clotrimazol	18A18-B05-347865	10
Fagron	Clotrimazol	18a18-b05-348429	1
Fagron	Clotrimazol	18A18-B05348429	1
Fagron	Clotrimazol	18A18-B05-348429	4
Fagron	Clotrimazol	18A18-B05-349662	5
Fagron	Clotrimazol	18A18-B05-3496662	1
Fagron	Clotrimazol	18A18-B05-350778	9
Fagron	Clotrimazol	18A18-B05350780	1
Fagron	Clotrimazol	18A18-B05-350780	7
Fagron	Clotrimazol	18A18-B05-350781	2
Fagron	Clotrimazol	18A18B05352114	1
Fagron	Clotrimazol	18A18-B05-352114	4
Fagron	Clotrimazol	18a18-b05-352115	1
Fagron	Clotrimazol	18A18-B05-352115	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazol	18A18B05353892	1
Fagron	Clotrimazol	18A18-B05-353892	5
Fagron	Clotrimazol	18A18-B05-355041	2
Fagron	Clotrimazol	18A18-B05-355042	1
Fagron	Clotrimazol	18G10-B06	6
Fagron	Clotrimazol	18G10-B06-352425	4
Fagron	Clotrimazol	18G10-B06-352426	2
Fagron	Clotrimazol	18G10-B06-352427	5
Fagron	Clotrimazol	18G10-B06352708	1
Fagron	Clotrimazol	18G10-B06-352708	5
Fagron	Clotrimazol	18G10-b06-353348	1
Fagron	Clotrimazol	18G10-B06-353348	4
Fagron	Clotrimazol	18G10-B06-354620	1
Fagron	Clotrimazol	18G10-B06-355382	2
Fagron	Clotrimazol	18G10-B06-355401	3
Fagron	Clotrimazol	18G10-B06-358825	12
Fagron	Clotrimazol	19/23-F06-367383	1
Fagron	Clotrimazol	1902004-01	1
Fagron	Clotrimazol	19814-B01-363547	2
Fagron	Clotrimazol	19B01363546	1
Fagron	Clotrimazol	19B14-B01	8
Fagron	Clotrimazol	19B14-B01_363546	1
Fagron	Clotrimazol	19B14-B01-259532	1
Fagron	Clotrimazol	19B14-B01-359531	6
Fagron	Clotrimazol	19b14-b01-359532	1
Fagron	Clotrimazol	19B14-B01-359532	5
Fagron	Clotrimazol	19b14-b01-359537	1
Fagron	Clotrimazol	19B14B01359537	1
Fagron	Clotrimazol	19B14-B01-359537	6
Fagron	Clotrimazol	19B14-B01-359538	3
Fagron	Clotrimazol	19B14-B01-359539	11
Fagron	Clotrimazol	19B14-B01-359540	1
Fagron	Clotrimazol	19b14-b01-361607	1
Fagron	Clotrimazol	19B14-B01-361607	8
Fagron	Clotrimazol	19B14-B01-361608	3
Fagron	Clotrimazol	19B14B01361609	1
Fagron	Clotrimazol	19B14-B01-361609	5
Fagron	Clotrimazol	19B14-B01-361610	1
Fagron	Clotrimazol	19B14-B01-363546	21
Fagron	Clotrimazol	19B14-B01-363546/4320	1
Fagron	Clotrimazol	19B14-B01-363547	10
Fagron	Clotrimazol	19B14-B01-363557	13
Fagron	Clotrimazol	19B14-B1-363557	1
Fagron	Clotrimazol	19B14-BO1-363557	1
Fagron	Clotrimazol	19J23	1
Fagron	Clotrimazol	19j23-06-367383	1
Fagron	Clotrimazol	19J23-F06_365713	1
Fagron	Clotrimazol	19J23-F06_367381	3
Fagron	Clotrimazol	19J23-F06-365713	10
Fagron	Clotrimazol	19J23-F06-3673803	2
Fagron	Clotrimazol	19J23-F06-367381	5
Fagron	Clotrimazol	19J23F06-367382	1
Fagron	Clotrimazol	19J23-F06-367382	7
Fagron	Clotrimazol	19j23-f06-367383	3
Fagron	Clotrimazol	19J23-F06367383	1
Fagron	Clotrimazol	19J23-F06-367383	14
Fagron	Clotrimazol	19J23-FO6-367383	2
Fagron	Clotrimazol	1A1-B05-34765	1
Fagron	Clotrimazol	2007033-01	1
Fagron	Clotrimazol	20111018	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazol	20120603	3
Fagron	Clotrimazol	20151112-3	1
Fagron	Clotrimazol	20170427Ma9	1
Fagron	Clotrimazol	20171127Ma1	1
Fagron	Clotrimazol	20B27-F02	4
Fagron	Clotrimazol	20B27-F02_369401	1
Fagron	Clotrimazol	20B27-F02-0369401	1
Fagron	Clotrimazol	20B27-F02-369401	9
Fagron	Clotrimazol	20B27-F02-369402	4
Fagron	Clotrimazol	20b27f02369403	1
Fagron	Clotrimazol	20B27F02369403	2
Fagron	Clotrimazol	20B27-F02-369403	7
Fagron	Clotrimazol	20B27F02-370980	1
Fagron	Clotrimazol	20B27-F02-370980	1
Fagron	Clotrimazol	20H19-F01	1
Fagron	Clotrimazol	20H19-F01_37345	1
Fagron	Clotrimazol	20H19-F01-373455	3
Fagron	Clotrimazol	20H19-F01-373456	8
Fagron	Clotrimazol	20H26-F05	6
Fagron	Clotrimazol	20H26-F05-3737302	1
Fagron	Clotrimazol	20H26-F05-373732	3
Fagron	Clotrimazol	20H26-F05-373733	1
Fagron	Clotrimazol	20H26-F05-373736	4
Fagron	Clotrimazol	20H26-F05-373737	1
Fagron	Clotrimazol	20h26-f05-373738	1
Fagron	Clotrimazol	20H26F05373738	1
Fagron	Clotrimazol	20H26-F05-373738	3
Fagron	Clotrimazol	20H26-F05-373739	2
Fagron	Clotrimazol	20H26-F05-373740	2
Fagron	Clotrimazol	20H26-F06	1
Fagron	Clotrimazol	20H26-F06-373736	1
Fagron	Clotrimazol	20OH26-F05-373739	1
Fagron	Clotrimazol	21/24-B11-213289	1
Fagron	Clotrimazol	21/24-B11-213289Fag	1
Fagron	Clotrimazol	21/24-B11-218638	1
Fagron	Clotrimazol	21124-B11-218638	1
Fagron	Clotrimazol	2124-B11	1
Fagron	Clotrimazol	21B12-B10-216242	1
Fagron	Clotrimazol	21D22-B03-217092	8
Fagron	Clotrimazol	21D22-B03-217713	1
Fagron	Clotrimazol	21H13B14213291	1
Fagron	Clotrimazol	21H13-B14213291	1
Fagron	Clotrimazol	21H13-B14-213291	11
Fagron	Clotrimazol	21I24-B11-213289	2
Fagron	Clotrimazol	21I24B11213292	1
Fagron	Clotrimazol	21I24-B11-213292	7
Fagron	Clotrimazol	21I24-B11-213293	1
Fagron	Clotrimazol	21I24-B11-218638	4
Fagron	Clotrimazol	21l24-B11	1
Fagron	Clotrimazol	21l24-B11-218638	1
Fagron	Clotrimazol	22A21-B02-217360	4
Fagron	Clotrimazol	22A21-B02-217361	2
Fagron	Clotrimazol	22A21-B02-221730	2
Fagron	Clotrimazol	22A21-BO2-217360	1
Fagron	Clotrimazol	23D11-B01-228693	1
Fagron	Clotrimazol	2616A-01276	1
Fagron	Clotrimazol	2OB27-FO2-369402	1
Fagron	Clotrimazol	2OB27-FO2-369403	1
Fagron	Clotrimazol	3716Q-01276	1
Fagron	Clotrimazol	4812E-01276(NP)	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazol	6C16MU1	1
Fagron	Clotrimazol	700120-0003	2
Fagron	Clotrimazol	700135-0003	1
Fagron	Clotrimazol	8556777	1
Fagron	Clotrimazol	9041304	1
Fagron	Clotrimazol	A21130J001	2
Fagron	Clotrimazol	B01-3616009	1
Fagron	Clotrimazol	B01-3635406	1
Fagron	Clotrimazol	B01-3635507	1
Fagron	Clotrimazol	B11-213289	1
Fagron	Clotrimazol	C22H17CIN2	1
Fagron	Clotrimazol	CLT/1307/0065A	2
Fagron	Clotrimazol	CLT/150570016b	1
Fagron	Clotrimazol	CLT/160/00058	1
Fagron	Clotrimazol	CLT/1604/00227A	1
Fagron	Clotrimazol	CLT/1604/0027A	2
Fagron	Clotrimazol	CLT/1607/0060A	2
Fagron	Clotrimazol	CLT/1709/0067B	1
Fagron	Clotrimazol	CLT/1711/0077A	2
Fagron	Clotrimazol	CLT/1805/00468	2
Fagron	Clotrimazol	CLT/1805/0046B	2
Fagron	Clotrimazol	CLT/1805/0064B	3
Fagron	Clotrimazol	CLT/1901/0002A	5
Fagron	Clotrimazol	CLT/2001/0006A	1
Fagron	Clotrimazol	CLT-1805-0046B	1
Fagron	Clotrimazol	F01-3734506	2
Fagron	Clotrimazol	F0236940001	1
Fagron	Clotrimazol	F02-3694001	4
Fagron	Clotrimazol	F02-3694002	1
Fagron	Clotrimazol	F02-3709800	1
Fagron	Clotrimazol	F05-3737302	1
Fagron	Clotrimazol	F06-3657103	1
Fagron	Clotrimazol	F06-3673801	2
Fagron	Clotrimazol	F06-3673803	3
Fagron	Clotrimazol	HCZ11520	4
Fargon/ Phoenix	Clotrimazol	18G10-B06-358825	1
Fargon/Noweda	Clotrimazol	18G-10-B06-355401	1
Fargon/Noweda	Clotrimazol	19B14-B01-363557	1
Fargon/Phönix	Clotrimazol	18147103	1
Fargon	Clotrimazol	16234511	1
Fargon	Clotrimazol	17J25-B06-345406	1
Fargon	Clotrimazol	18A18-B05-350778	1
Fargon	Clotrimazol	18g10-b06-355401	1
Fargon	Clotrimazol	18G10-B06-355401	1
Fargon	Clotrimazol	19B14-B01-363547	1
Fargon	Clotrimazol	20B27-F02-369403	1
Fargron / Noweda	Clotrimazol	16E20-B10-324555	1
Fiebig 10.06.13 ek: 8,58EUR	Clotrimazol	12E30-N07	1
Fiebig	Clotrimazol	1607046-01	1
Fiebig	Clotrimazol	1607046-02	1
Fiebig	Clotrimazol	1703028	1
Fiebig	Clotrimazol	1703028-03	1
Fiebig	Clotrimazol	1808028-02	1
Fiebig	Clotrimazol	18147101	1
Fiebig	Clotrimazol	20000092006	1
Fiebig	Clotrimazol	20000094008	1
Finteler Apotheke	Clotrimazol	16234501	1
Finteler Apotheke	Clotrimazol	16234509	1
Fischar/Gehe	Clotrimazol	20111018	1
Fragon	Clotrimazol	19B14-B01-363557	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fragon	Clotrimazol	21H13-B14-218610	1
Fragron/noweda	Clotrimazol	17A19-B04	1
Fragron/noweda	Clotrimazol	CLT/1601/0005B	1
Gatt-Koller	Clotrimazol	1801870	1
Gatt-Koller	Clotrimazol	201714s9	1
Gehe amax	Clotrimazol	14B05-B35-294935	1
Gehe amax	Clotrimazol	1607046-02	1
Gehe amax	Clotrimazol	16J07-B02-330216	1
Gehe amax	Clotrimazol	17111608	1
Gehe amax	Clotrimazol	1808028-01	1
Gehe amax	Clotrimazol	19J23-F06-365713	1
Gehe amax	Clotrimazol	20000092005	1
Gehe	Clotrimazol	1108053-01	1
Gehe	Clotrimazol	11K21-N19	1
Gehe	Clotrimazol	12/21-N01	1
Gehe	Clotrimazol	121003902	1
Gehe	Clotrimazol	1306036-01	3
Gehe	Clotrimazol	1309034-01	1
Gehe	Clotrimazol	13184103	1
Gehe	Clotrimazol	13224216	1
Gehe	Clotrimazol	1409027-02	2
Gehe	Clotrimazol	14337815	2
Gehe	Clotrimazol	14337819	1
Gehe	Clotrimazol	14B05B35294935	1
Gehe	Clotrimazol	14B05-B35-294935	1
Gehe	Clotrimazol	14C04-B31-294952	1
Gehe	Clotrimazol	15G14-B05	1
GEHE	Clotrimazol	1607046-02	1
Gehe	Clotrimazol	16234505	1
Gehe	Clotrimazol	16234511	1
Gehe	Clotrimazol	16234513	1
GEHE	Clotrimazol	16234513	1
Gehe	Clotrimazol	16E20-B10-321598	2
GEHE	Clotrimazol	16J07-B02	1
Gehe	Clotrimazol	16j07-b02-330216	1
Gehe	Clotrimazol	16J07-B02-330216	1
Gehe	Clotrimazol	1703028-02	1
Gehe	Clotrimazol	17111603	1
Gehe	Clotrimazol	17111605	1
Gehe	Clotrimazol	17111616	1
Gehe	Clotrimazol	17360201	1
GEHE	Clotrimazol	17360202	1
GEHE	Clotrimazol	177111613	1
Gehe	Clotrimazol	17A19-B04	1
Gehe	Clotrimazol	17A19-B04-338560	1
Gehe	Clotrimazol	17J25-B06-0345044	1
Gehe	Clotrimazol	17J25-B06-345048	1
Gehe	Clotrimazol	17J25-B06-345407	1
Gehe	Clotrimazol	1808028-01	4
Gehe	Clotrimazol	1808028-02	1
Gehe	Clotrimazol	18147101	1
Gehe	Clotrimazol	18147103	1
GEHE	Clotrimazol	18147103	1
GEHE	Clotrimazol	18147210	2
Gehe	Clotrimazol	18A18-B05-350778	1
Gehe	Clotrimazol	18G10-B06	2
Gehe	Clotrimazol	18G10-B06-0046B	1
Gehe	Clotrimazol	18G10-B06-358825	1
Gehe	Clotrimazol	19016106	1
Gehe	Clotrimazol	19016108	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Clotrimazol	19016116	1
Gehe	Clotrimazol	1902004-02	2
Gehe	Clotrimazol	1902004-03	2
Gehe	Clotrimazol	200000094004	1
gehe	Clotrimazol	20000092002	1
Gehe	Clotrimazol	20000092006	1
Gehe	Clotrimazol	20000094003	2
Gehe	Clotrimazol	20000094006	1
Gehe	Clotrimazol	2007033-02	1
Gehe	Clotrimazol	21000123006	2
Gehe	Clotrimazol	21004116005	1
Gehe	Clotrimazol	21004116007	2
Gehe	Clotrimazol	21004116013	1
Gehe	Clotrimazol	21004116014	3
gehe	Clotrimazol	21004116016	1
Gehe	Clotrimazol	21004117003	1
Gehe	Clotrimazol	21004117007	1
Gehe	Clotrimazol	21004117016	1
Gehe	Clotrimazol	21004117018	1
Gehe	Clotrimazol	2103021-01	1
Gehe	Clotrimazol	2103024-01	1
Gehe	Clotrimazol	22A21-B02-217361	1
GEHE	Clotrimazol	23001596002	1
Gehe	Clotrimazol	23001596008	2
Gehe	Clotrimazol	2301055-01	1
Gehe	Clotrimazol	CLT/1805/0046B	1
Gehe	Clotrimazol	HCZ14218	1
Geilenkirchen	Clotrimazol	17360204	1
Geilenkirchen	Clotrimazol	20000094004	1
Guangzhou Hanpu Phar...	Clotrimazol	14337819	1
Guangzhou Hanpu Phar...	Clotrimazol	1409027-03	1
Guangzhou Hanpu Phar...	Clotrimazol	1510003-01	1
Guangzhou Hanpu Phar...	Clotrimazol	1510003-02	1
Guangzhou Hanpu Pharmac.	Clotrimazol	1703028-02	1
Halcycon Labs	Clotrimazol	19016104	1
Halcyon / Noweda	Clotrimazol	18147210	1
Halcyon Labs / Gehe ...	Clotrimazol	18147103	1
Halcyon Labs Pvt. Lt...	Clotrimazol	20000094006	1
Halcyon Labs Pvt.Ltd...	Clotrimazol	W8269	1
Halcyon Labs Pvt.Ltd...	Clotrimazol	18147101	1
Halcyon Labs Pvt	Clotrimazol	20003904004	1
Halcyon Labs/	Clotrimazol	19016105	1
Halcyon Labs	Clotrimazol	1808028-02	1
Halcyon Labs	Clotrimazol	20000094005	1
Halcyon/Link & Eccius	Clotrimazol	W8269	1
Halcyon/Noweda	Clotrimazol	20000094008	1
Halcyon/Noweda	Clotrimazol	HCZ14518	1
Halcyon/Noweda	Clotrimazol	HCZ14718	1
Halycon Labs / Fiebig	Clotrimazol	HCZ06718	1
Hedinger/Alliance H.	Clotrimazol	15395617	2
Hedinger/Gehe	Clotrimazol	1703028-02	1
Henry Lamotte oils GmbH	Clotrimazol	18147203	1
Jenne	Clotrimazol	18147103	1
Jenne	Clotrimazol	20000092006	1
JENNE	Clotrimazol	21004116007	1
Jenne	Clotrimazol	23001596009	2
Jenne	Clotrimazol	2301055-01	1
Kehr	Clotrimazol	1808028-01	1
Kehr	Clotrimazol	18g10-b06-3533348	1
Kehr	Clotrimazol	18g10-b06-353348	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Clotrimazol	21004116013	1
Kehr	Clotrimazol	21004116014	1
Kehr	Clotrimazol	21004117022	1
Kehr	Clotrimazol	2103024-02	1
Kehr	Clotrimazol	2301055-01	2
Klenk	Clotrimazol	16B09-B06-311785	1
Klosterring	Clotrimazol	16234512	1
Klosterring	Clotrimazol	17111615	2
Klosterring	Clotrimazol	6234505	1
L12	Clotrimazol	16234512	1
L12	Clotrimazol	17111606	1
L12	Clotrimazol	17360204	1
Link &Eccius (Halcyo…	Clotrimazol	W8269	1
Maros Arznei GmbH	Clotrimazol	13184105	1
Martin Apo	Clotrimazol	31117/1	1
Midas	Clotrimazol	1703028-01	1
Midas	Clotrimazol	1703028-03	1
Midas	Clotrimazol	1808028-02	1
Mvda_15.01.2019	Clotrimazol	18147102	1
Nachprüfung	Clotrimazol	2082019-4	1
Noveda	Clotrimazol	20003904003	1
Noweda 06.11.2019	Clotrimazol	19016119	1
Noweda 07.07.2015	Clotrimazol	14144913	1
Noweda 17.7.2019	Clotrimazol	19016105	1
Noweda Fiebig 15.05.…	Clotrimazol	20000092002	1
Noweda Taucha	Clotrimazol	19016206	1
Noweda/EuRho	Clotrimazol	2103024-01	1
Noweda/Fargon	Clotrimazol	17A19-B04-336568	1
Noweda	Clotrimazol	1203040-03	2
Noweda	Clotrimazol	13224201	1
Noweda	Clotrimazol	13224217	1
Noweda	Clotrimazol	1409027	1
Noweda	Clotrimazol	1409027-02	1
Noweda	Clotrimazol	14337801	1
Noweda	Clotrimazol	14337816	1
Noweda	Clotrimazol	1510003-01	2
Noweda	Clotrimazol	15G14-B05-316483	2
Noweda	Clotrimazol	16234511	3
Noweda	Clotrimazol	16234517	2
Noweda	Clotrimazol	16J07-B02-329386	1
Noweda	Clotrimazol	16j07-b02-341842	1
Noweda	Clotrimazol	1703028-01	1
Noweda	Clotrimazol	17111608	1
Noweda	Clotrimazol	17360201	1
Noweda	Clotrimazol	17360203	2
Noweda	Clotrimazol	17J25-B06-345044	1
Noweda	Clotrimazol	18147203	2
Noweda	Clotrimazol	18147211	1
Noweda	Clotrimazol	18147212	1
Noweda	Clotrimazol	18A18-B05	1
Noweda	Clotrimazol	18G10-B06	1
Noweda	Clotrimazol	18G10-B06-352425	1
Noweda	Clotrimazol	18G10-B06-358825	2
Noweda	Clotrimazol	19016104	1
Noweda	Clotrimazol	19016107	1
Noweda	Clotrimazol	19016202	2
Noweda	Clotrimazol	19016204	1
Noweda	Clotrimazol	19016208	1
Noweda	Clotrimazol	19020004-01	1
Noweda	Clotrimazol	1902004_01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Clotrimazol	1902004-02	1
Noweda	Clotrimazol	19B14-B01-359539	1
Noweda	Clotrimazol	20000094005	1
Noweda	Clotrimazol	2007033-01	1
Noweda	Clotrimazol	2007033-02	2
Noweda	Clotrimazol	20111115	1
Noweda	Clotrimazol	20H26-F05-373738	1
Noweda	Clotrimazol	20H26-F05-373739	4
Noweda	Clotrimazol	21000121002	1
Noweda	Clotrimazol	21000123008	1
Noweda	Clotrimazol	21000123011	1
Noweda	Clotrimazol	21004116013	1
Noweda	Clotrimazol	21004117001	1
Noweda	Clotrimazol	21004117018	2
Noweda	Clotrimazol	21004117019	2
Noweda	Clotrimazol	2103024-01	1
Noweda	Clotrimazol	2103024-03	1
Noweda	Clotrimazol	21H13-B14-213291	2
Noweda	Clotrimazol	22A21-B02-221730	1
Noweda	Clotrimazol	2301055-01	1
Oberlinden Apotheke	Clotrimazol	201401300378	2
p&m cosmetics/gehe	Clotrimazol	16J07-B02-335773	2
Phö/Dr.Wolff	Clotrimazol	19016108	1
Phoenix 23.10.14 5,50	Clotrimazol	1309034-02	1
Phoenix 24.04.2017	Clotrimazol	1607046-02	1
PHOENIX am 22.01.2014	Clotrimazol	1306036-01	1
Phoenix	Clotrimazol	12A05-N10	1
Phoenix	Clotrimazol	1309034-02	1
Phoenix	Clotrimazol	13224215	1
Phoenix	Clotrimazol	14337812	1
Phoenix	Clotrimazol	14c04b31	1
Phoenix	Clotrimazol	1607046-01	1
Phoenix	Clotrimazol	16234509	1
phoenix	Clotrimazol	16234512	1
Phoenix	Clotrimazol	16B11-B04-327611	1
Phoenix	Clotrimazol	17111601	1
Phoenix	Clotrimazol	17111603	1
Phoenix	Clotrimazol	18147102	1
Phoenix	Clotrimazol	1902004-01	1
Phoenix	Clotrimazol	1902004-02	2
Phoenix	Clotrimazol	191381012	1
Phoenix	Clotrimazol	20000092006	1
Phoenix	Clotrimazol	20000094003	1
Phoenix	Clotrimazol	20003904004	1
Phoenix	Clotrimazol	21000121002	1
phoenix	Clotrimazol	21000121004	3
Phoenix	Clotrimazol	21000121006	1
Phoenix	Clotrimazol	21004116014	1
Phoenix	Clotrimazol	21004117004	1
Phoenix	Clotrimazol	21004117016	1
Phoenix	Clotrimazol	21004117017	1
Phoenix	Clotrimazol	2103024-02	1
Phoenix	Clotrimazol	22A21-B02-217361	1
Phoenix	Clotrimazol	23001596002	1
Phoenix	Clotrimazol	2301055-01	1
Phoenix	Clotrimazol	3088	1
Phoenix	Clotrimazol	3237	1
Phoenix	Clotrimazol	79879	1
Phönix Gotha	Clotrimazol	14337811	1
Phönix Gotha	Clotrimazol	16J07-B02-344816	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix WE:23.10.17 …	Clotrimazol	16234521	1
Phönix	Clotrimazol		1
phönix	Clotrimazol	11305513	1
Phönix	Clotrimazol	13C25-N10	1
Phönix	Clotrimazol	1409027-01	1
phönix	Clotrimazol	14337818	1
Phönix	Clotrimazol	15395618	1
Phönix	Clotrimazol	1607046-01	1
Phönix	Clotrimazol	16234505	1
phönix	Clotrimazol	16234512	1
phönix	Clotrimazol	16B11-B04-327611	1
Phönix	Clotrimazol	1703028-03	1
Phönix	Clotrimazol	17111603	1
Phönix	Clotrimazol	17111604	1
Phönix	Clotrimazol	17111608	2
Phönix	Clotrimazol	17360203	1
Phönix	Clotrimazol	18147103	1
Phönix	Clotrimazol	18147203	1
PHÖNIX	Clotrimazol	18147203	1
Phönix	Clotrimazol	18147212	1
Phönix	Clotrimazol	18G10-B06-354620	2
Phönix	Clotrimazol	19016104	1
Phönix	Clotrimazol	19016108	1
Phönix	Clotrimazol	19016116	1
Phönix	Clotrimazol	19016203	1
Phönix	Clotrimazol	19016205	1
Phönix	Clotrimazol	1902004-01	2
Phönix	Clotrimazol	1902004-02	1
Phönix	Clotrimazol	1902004-03	2
PHÖNIX	Clotrimazol	19b14b01363546	1
Phönix	Clotrimazol	20000092007	1
Phönix	Clotrimazol	2007033-01	1
PHÖNIX	Clotrimazol	200703301	1
Phönix	Clotrimazol	2007033-03	1
Phönix	Clotrimazol	200742407	1
Phönix	Clotrimazol	201033-01	1
Phönix	Clotrimazol	20160801	1
Phönix	Clotrimazol	21000121002	1
Phönix	Clotrimazol	21004116007	2
Phönix	Clotrimazol	21004116013	1
Phönix	Clotrimazol	21004116016	1
Phönix	Clotrimazol	21004117022	1
Phönix	Clotrimazol	2103024-01	1
Phönix	Clotrimazol	23001596002	2
Phönix	Clotrimazol	23001596003	2
Phönix	Clotrimazol	23003390001	1
Röntgen	Clotrimazol	1703028-01	5
Röntgen	Clotrimazol	1808028-01	3
Röntgen	Clotrimazol	1902004-03	1
Röntgen	Clotrimazol	2007033-02	1
Röntgen	Clotrimazol	2103024-01	1
Sanacorp/Caela	Clotrimazol	17111603	1
Sanacorp	Clotrimazol	105/AKD1	1
Sanacorp	Clotrimazol	109/AKD3	1
Sanacorp	Clotrimazol	109/AKD6	1
Sanacorp	Clotrimazol	1203040-03	1
Sanacorp	Clotrimazol	12159902	1
Sanacorp	Clotrimazol	1230805	1
Sanacorp	Clotrimazol	12320814	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Clotrimazol	13184105	1
Sanacorp	Clotrimazol	13224214	2
Sanacorp	Clotrimazol	13224219	1
Sanacorp	Clotrimazol	14144905	1
sanacorp	Clotrimazol	14144918	1
Sanacorp	Clotrimazol	14337817	1
Sanacorp	Clotrimazol	15g14-b05-311100	1
Sanacorp	Clotrimazol	16E20-B10-327349	1
Sanacorp	Clotrimazol	16J07-B02-330216	1
Sanacorp	Clotrimazol	16J07-B02-338283	1
Sanacorp	Clotrimazol	1703028-02	1
Sanacorp	Clotrimazol	170302803	1
Sanacorp	Clotrimazol	17360201	1
Sanacorp	Clotrimazol	17360203	1
Sanacorp	Clotrimazol	18147102	1
Sanacorp	Clotrimazol	18147210	2
Sanacorp	Clotrimazol	18147211	1
Sanacorp	Clotrimazol	18147212	1
Sanacorp	Clotrimazol	1882321	1
Sanacorp	Clotrimazol	18G10-B06	1
Sanacorp	Clotrimazol	19016116	1
Sanacorp	Clotrimazol	19016203	3
Sanacorp	Clotrimazol	19016208	2
Sanacorp	Clotrimazol	19B14-B01-359537	1
Sanacorp	Clotrimazol	20000094006	1
Sanacorp	Clotrimazol	20000094008	1
sanacorp	Clotrimazol	20003904004	1
Sanacorp	Clotrimazol	20003904005	1
Sanacorp	Clotrimazol	200703302	1
Sanacorp	Clotrimazol	20H19-F01	1
Sanacorp	Clotrimazol	20H26-F05	1
Sanacorp	Clotrimazol	21000121006	2
Sanacorp	Clotrimazol	21000123008	1
Sanacorp	Clotrimazol	21000123010	1
Sanacorp	Clotrimazol	21004116013	1
Sanacorp	Clotrimazol	21004116014	2
Sanacorp	Clotrimazol	21004116017	1
sanacorp	Clotrimazol	21004117005	1
Sanacorp	Clotrimazol	21D22-B03-217092	2
Sanacorp	Clotrimazol	21H13-B14-213291	1
Sanacorp	Clotrimazol	22A21-B02-221671	1
Sanacorp	Clotrimazol	23001596003	1
sanacorp	Clotrimazol	2301055-01	1
Sanacorp	Clotrimazol	APCLT/1703/0016CC	1
Sino Phyto	Clotrimazol	13224210	2
Stumpf	Clotrimazol	12159902	1
Vdl 14.07.14	Clotrimazol	13224225	1
VDL;11.06.15;27,90EUR	Clotrimazol	14337807	1
WE Phönix.01.12.2016. . .	Clotrimazol	15395618	1
wepa/Sanaco	Clotrimazol	14337819	1

- 229 124 spectra from 1515 *Apo-Ident* customers from a total of 48 342 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Clotrimazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clotrimazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	640	0	201 444
Type C	0	6858	85	229 124

The substance/substance group *Clotrimazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0625 %)
Type C	100.0000 % (> 99.9007 %)	98.7757 % (> 98.7325 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20794	22229	6,09	60,32
21087	23791	9,03	62,60
21114	23791	8,80	59,16
21207	25649	7,34	54,96
21259	25649	10,25	57,55
21264	25656	4,66	55,46
21352	22229	8,41	59,45
21353	22229	8,88	59,06
22229	22229	0,00	63,00
23791	23791	0,00	57,61
25649	25649	0,00	52,59
25656	25656	0,00	53,46
26137	25656	25,97	47,16

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Colesterol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20446-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Colesterol; Cholesterolum

Special notes

When selecting the *Colesterol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Colesterol	8	5	176

Second-stage model

For differentiation of the substance/substance group *Colesterol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Colesterol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Álcoois de cera de lã	72,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Colesterol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Colesterol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Colesterol	160444	22461	60	20160222*
Caelo	Colesterol	16044415	23760	40	1804387
Caelo	Colesterol	21000039004	25517	40	20210127
Caelo	Colesterol	23002121	26963	40	20230922*
Caelo	Colesterol	23002121	26963SI	20	20230922*
Fagron	Colesterol	13F10-B40	21219	40	20131223
Fagron	Colesterol	15J23-B03-325106	22971	40	20151103
Fagron	Colesterol	17E17-B05-339074	23937	40	20170620
Fagron	Colesterol	22D05-B03-220575	26160	40	20220519
Fagron	Colesterol	22D05-B03-220575	26160SI	20	20220519

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Colesterol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 582 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 6 reference samples from the substance/substance group *Colesterol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Colesterol	13148703	21310	40
Caelo	Colesterol	190549	24712	40
Caelo	Colesterol	22001179	26111	40
Fagron	Colesterol	16G05-B03-331396	23522	40
Fagron	Colesterol	24D26-B01-240098	27424	40
Caelo	Colesterol	22001179	26111SI	20

- 201 864 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 442 spectra from 165 *Apo-Ident* customers from 184 batches from the substance/substance group *Colesterol*.

- Among them are spectra of independent samples from 175 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Colesterol	22001179013	1
	Colesterol	2203-B01-229435	1
	Colesterol	22D05-B03-220341	1
	Colesterol	22J03-B01	1
	Colesterol	22j03b01224448	1
	Colesterol	22j03-b01-224452	1
	Colesterol	22J03-B01-229435	4
	Colesterol	23D21-B03-229928	1
	Colesterol	41172	2
	Colesterol	B01-2244502	1
	Colesterol	B01-2386705	2
AHD	Colesterol	17K16-B11-352718	1
Anzag/Fargon	Colesterol	19J18-B02	1
Caelo	Colesterol	11242103	1
Caelo	Colesterol	12155605	1
Caelo	Colesterol	12248403	1
Caelo	Colesterol	13056903	1
Caelo	Colesterol	13148704	1
Caelo	Colesterol	14027201	1
Caelo	Colesterol	14122501	2
Caelo	Colesterol	14208602	1
Caelo	Colesterol	15028303	1
Caelo	Colesterol	15301803	3
Caelo	Colesterol	15358801	5
Caelo	Colesterol	15407101	2
Caelo	Colesterol	15407102	2
Caelo	Colesterol	15B09-B02-308259	1
Caelo	Colesterol	15G31-B05-312376	1
Caelo	Colesterol	15J23-B03	1
Caelo	Colesterol	15J23-B03_329505	1
Caelo	Colesterol	16044402	1
Caelo	Colesterol	16044407	4
Caelo	Colesterol	16044408	2
Caelo	Colesterol	16044409	2
Caelo	Colesterol	16044413	4
Caelo	Colesterol	16044415	4
Caelo	Colesterol	16044416	6
Caelo	Colesterol	16G05-B03	1
Caelo	Colesterol	17K16-B11-343922	1
Caelo	Colesterol	17K16-B11-345814	1
Caelo	Colesterol	17K16-B11-348760	1
Caelo	Colesterol	17K16-B11-350557	2
Caelo	Colesterol	18097102	2
Caelo	Colesterol	18097202	2
Caelo	Colesterol	19054901	7
Caelo	Colesterol	19054903	6
Caelo	Colesterol	191949001	2
Caelo	Colesterol	191949003	2
Caelo	Colesterol	19194902	4
Caelo	Colesterol	19194903	2
Caelo	Colesterol	19194904	9
Caelo	Colesterol	19I18-B02	1
Caelo	Colesterol	19I20-B08	1
Caelo	Colesterol	19J18-B02-201592	1
Caelo	Colesterol	19J18-B01-201136	1
Caelo	Colesterol	20G08-B02	1
Caelo	Colesterol	20G08-B02-202266	3
Caelo	Colesterol	21000039004	2
Caelo	Colesterol	21000039006	4
Caelo	Colesterol	21000039009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Colesterol	2100039009	1
Caelo	Colesterol	21C18-B01-213585	2
Caelo	Colesterol	21F08-B20-215610	1
Caelo	Colesterol	22001179004	1
Caelo	Colesterol	27212	1
Caelo	Colesterol	32124	1
Caelo	Colesterol	B02-2015901	1
Caesar & Loretz GmbH	Colesterol	18097202	1
Caesar & Loretz GmbH	Colesterol	19194903	2
Ebert-Jacobi	Colesterol	16044408	1
Ensbona /Alliance He...	Colesterol	17E17-B05-339074	3
Euro OTC	Colesterol	13F10-B40-289016	1
Fagro/EJ	Colesterol	17K16-B11_348760	1
Fagron	Colesterol		1
Fagron	Colesterol	10B15-N07	1
Fagron	Colesterol	10H24-N06	1
Fagron	Colesterol	11A17-N07	1
Fagron	Colesterol	1213585	1
Fagron	Colesterol	12D02-N10	1
Fagron	Colesterol	12I13-N02	2
Fagron	Colesterol	13C25-N12	2
Fagron	Colesterol	13F10-B40	1
Fagron	Colesterol	13F10-B40-289016	2
Fagron	Colesterol	13G10-N11	3
Fagron	Colesterol	14B27-B05	2
Fagron	Colesterol	14B27-B05-293548	3
Fagron	Colesterol	14B27-B05-293550	1
Fagron	Colesterol	14G04-B02	1
Fagron	Colesterol	14G04-B02-300830	2
Fagron	Colesterol	14G04-B02-300831	1
Fagron	Colesterol	15B09	1
Fagron	Colesterol	15B09-B02	1
Fagron	Colesterol	15B09-B02-308259	4
Fagron	Colesterol	15B09-B02-308847	2
Fagron	Colesterol	15G31-B05	2
Fagron	Colesterol	15G31-B05_316721	1
Fagron	Colesterol	15G31-B05-312377	1
Fagron	Colesterol	15G31-B05-312378	1
Fagron	Colesterol	15G31-B05-314182	2
Fagron	Colesterol	15G31-B05-316721	3
Fagron	Colesterol	15J23-B03	1
Fagron	Colesterol	15J23B03320483	1
Fagron	Colesterol	15J23-B03-320483	5
Fagron	Colesterol	15J23B03322902	1
Fagron	Colesterol	15J23-B03-322902	1
Fagron	Colesterol	15j23-B03-325106	1
Fagron	Colesterol	15J23B03325106	1
Fagron	Colesterol	15J23-B03-325106	5
Fagron	Colesterol	15J23B03328249	1
Fagron	Colesterol	15J23-B03-328249	2
Fagron	Colesterol	16G05-B03	1
Fagron	Colesterol	16G05-B03-331396	2
Fagron	Colesterol	16G05-B03-331397	1
Fagron	Colesterol	16G05-B03-333996	3
Fagron	Colesterol	16G05-B03-334366	1
Fagron	Colesterol	16GB05-B03	1
Fagron	Colesterol	17E17-B05	2
Fagron	Colesterol	17E17-B05-337588	5
Fagron	Colesterol	17E17-B05-339074	5
Fagron	Colesterol	17E17-B05-339075	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Colesterol	17K16-B11-343922	3
Fagron	Colesterol	17K16-B11-343923	1
Fagron	Colesterol	17K16-B11-345814	2
Fagron	Colesterol	17K16-B11-348760	4
Fagron	Colesterol	17K16-B11-348761	3
Fagron	Colesterol	17K16-B11-348762	1
Fagron	Colesterol	17K16-B11-349922	1
Fagron	Colesterol	17K16B11350557	1
Fagron	Colesterol	17K16-B11-350557	6
Fagron	Colesterol	17K16-B11-352718	13
Fagron	Colesterol	17K16-B11-355385	7
Fagron	Colesterol	17k16-B11-43922	1
Fagron	Colesterol	18I03-B06	1
Fagron	Colesterol	18I03-B06-353374	2
Fagron	Colesterol	18I03-B06-355386	1
Fagron	Colesterol	18I03-B06-356700	1
Fagron	Colesterol	18J18-B02-201591	1
Fagron	Colesterol	19120B08200506	1
Fagron	Colesterol	19120-B08-200506	2
Fagron	Colesterol	19120-BO8-200506	1
Fagron	Colesterol	1920B0B-200561	1
Fagron	Colesterol	19E20-B02-191413	1
Fagron	Colesterol	19E20-B02-192819	2
Fagron	Colesterol	19G12-B0313-194214	1
Fagron	Colesterol	19g12-b13-194214	1
Fagron	Colesterol	19G12-B13-194214	8
Fagron	Colesterol	19G12-B13-194216	1
Fagron	Colesterol	19I20-B08	2
Fagron	Colesterol	19I20-B08-196479	4
Fagron	Colesterol	19I20-B08-196480	1
Fagron	Colesterol	19I20-B08-200506	6
Fagron	Colesterol	19I20-B08-200559	2
Fagron	Colesterol	19I20-B08-200561	4
Fagron	Colesterol	19J18-B01-201136	5
Fagron	Colesterol	19J18-B02	1
Fagron	Colesterol	19J18B02196477	1
Fagron	Colesterol	19J18-B02-196477	8
Fagron	Colesterol	19J18-B02-201591	5
Fagron	Colesterol	19J18-B02-201592	1
Fagron	Colesterol	19j18-BO2	1
Fagron	Colesterol	19j18-bo2-201595	1
Fagron	Colesterol	19J19-B02-201592	1
Fagron	Colesterol	19l20-B08-196480	1
Fagron	Colesterol	2013U-01270	1
Fagron	Colesterol	20F25-B99-201594	3
Fagron	Colesterol	20G08-0B02-202266	1
Fagron	Colesterol	20G08-B02	4
Fagron	Colesterol	20G08-B02-201946	6
Fagron	Colesterol	20G08-B02-202265	5
Fagron	Colesterol	20G08-B02-202266	9
Fagron	Colesterol	20G08-B02-202266	1
Fagron	Colesterol	20G08-BO2-201946	1
Fagron	Colesterol	20G08-N02-202265	1
Fagron	Colesterol	21c18B01213585	1
Fagron	Colesterol	21C18B01213585	2
Fagron	Colesterol	21C18-B01-213585	14
Fagron	Colesterol	21C18-B01-213586	1
Fagron	Colesterol	21C18-BO1	1
Fagron	Colesterol	21F08-b20-213589	1
Fagron	Colesterol	21FO8-B20	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Colesterol	22d05-b03-220495	1
Fagron	Colesterol	22J03-B01-224448	2
Fagron	Colesterol	27212	1
Fagron	Colesterol	20G08-B02-202266	1
Fagron	Colesterol	30197	1
Fagron	Colesterol	30969	2
Fagron	Colesterol	31941	2
Fagron	Colesterol	322124	1
Fagron	Colesterol	34342	4
Fagron	Colesterol	36062	2
Fagron	Colesterol	8J28-N10	1
Fagron	Colesterol	B01-2011306	1
Fagron	Colesterol	B02_2022606	1
Fagron	Colesterol	B02-1964707	1
Fagron	Colesterol	B02-2015901	1
Fagron	Colesterol	B02-2015905	1
Fagron	Colesterol	B02-2022606	6
Fagron	Colesterol	B20-2135809	1
Fargon / AHD	Colesterol	16G05-B03-334366	1
Fargon/Alliance	Colesterol	21C18-B01-213585	2
Fargon/AllianceH.	Colesterol	16G05-B03-328689	1
Fargon	Colesterol	19G12-B13-194214	1
Gehe	Colesterol	B02-2019406	1
Noweda	Colesterol	15358802	1
Noweda	Colesterol	15J23-B03-320483	1
Noweda	Colesterol	17K16-B11-343922	2
Noweda	Colesterol	19194904	3
Noweda	Colesterol	22001179013	1
Phönix/Fargon	Colesterol	17K16-B11-355385	1
Phönix	Colesterol	19G-12-B13-194214	1
Phönix	Colesterol	1K16-B11-343922	1
Sanacorp	Colesterol	21000039010	1
Sanacorp	Colesterol	22J03-B01-229435	1
Sanacorp	Colesterol	23003286002	1

- 235 625 spectra from 1515 *Apo-Ident* customers from a total of 49 075 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Colesterol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Colesterol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	220	0	201 864
Type C	0	439	3	235 625

The substance/substance group *Colesterol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9007 %)	99.3213 % (> 98.6425 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21219	23760	6,80	125,28
22461	22461	0,00	126,44
22971	22461	21,86	125,39
23760	23760	0,00	123,67
23937	23760	23,00	125,84
25517	22461	8,45	124,43
26160	22461	15,11	125,57
26963	26963	0,00	122,80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Concentrado seco de acetato de alfa-tocoferol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20433-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Concentrado seco de acetato de alfa-tocoferol; Acetato de Racealfatocoferol 50%; Alfa-tocoferol - acetato 50%; DL-alfa-tocoferol acetato 50%; Vitamina E acetato pó 50%

Special notes

When selecting the *Concentrado seco de acetato de alfa-tocoferol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Concentrado seco de acetato de alfa-tocoferol	10	10	23

Second-stage model

For differentiation of the substance/substance group *Concentrado seco de acetato de alfa-tocoferol* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Concentrado seco de acetato de alfa-tocoferol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Nistatina	64,60	27,61
⋮	⋮	⋮
Bacitracina	>50	18,72
Anfotericina B	>50	35,80
Sulfato de polimixina B	76,78	41,80
Sulfato de colistina	>50	46,14
Levedura de selênio	>50	50,17
Cianocobalamina	>50	53,39
Estriol	>50	62,11
Estradiol hemi-hidratado	>50	63,89
Riboflavina	>50	68,54
Glicerofosfato de cálcio	>50	77,14
Triancinolona	>50	91,34
Carmelose sódica	>50	101,48
Pantotenato de cálcio	>50	122,62
Gelatina, branca	>50	145,58
Metilcobalamina	>50	169,20
SyrSpend® SF Alka	>50	178,21
Bromidrato de hioscina	>50	181,97
SyrSpend® SF pH4 neo	>50	185,88
Tosilcloramida sódica	>50	187,50
Amido de arroz	>50	201,70
Amido de milho	>50	263,04
Ácido oxálico	>50	281,34
SyrSpend® SF pH4	>50	342,55
Goma arábica, dispersão seca	>50	370,10
Maltodextrina	>50	376,64
Amido de trigo	>50	399,60
Fécula de batata	>50	417,15
Frutose	>50	631,69

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Concentrado seco de acetato de alfa-tocoferol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Concentrado seco de acetato de alfa-tocoferol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Concentrado seco de aceta…	1110021-02	20907	40	20120104
Euro OTC	Concentrado seco de aceta…	1305032-01	21680	60	AR-15-FG-001194-01
Euro OTC	Concentrado seco de aceta…	1507001	21842	60	20130708*
Euro OTC	Concentrado seco de aceta…	1603046	22543	40	20160429*
Euro OTC	Concentrado seco de aceta…	1907033	24841	40	20190820*
Euro OTC	Concentrado seco de aceta…	2005022	25277	40	20200728*
Euro OTC	Concentrado seco de aceta…	2101019	25599	40	20210323*
Fagron	Concentrado seco de aceta…	13H30-B02-287169	21609	60	AR-15-FG-006388-01
Fagron	Concentrado seco de aceta…	14B03-B04-295113	21959	60	20140224
Fagron	Vitamina E acetato pó 50%	022402A013	BR20042	40	20240919*
Fagron	Vitamina E acetato pó 50%	022402A013	BR20042SI	20	20240919*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 500 spectra of 11 reference samples from the substance/substance group *Concentrado seco de acetato de alfa-tocoferol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 462 spectra from a total of 2832 batches from further 484 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 510 spectra of 15 reference samples from the substance/substance group *Concentrado seco de acetato de alfa-tocoferol*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Concentrado seco de aceta…	1705003	23424	40
Euro OTC	Concentrado seco de aceta…	1810024	24309	40
Euro OTC	Concentrado seco de aceta…	2106013	25780	50
Euro OTC	Concentrado seco de aceta…	2111015	25889	50
Euro OTC	Concentrado seco de aceta…	2207013	26279	40
Euro OTC	Concentrado seco de aceta…	2309007	26929	40
Euro OTC	Concentrado seco de aceta…	2408017	27395	40
Fagron	Concentrado seco de aceta…	16H30-B05-326792	22948	40
Fagron	Vitamina E acetato pó 50%	022403A011	BR20041	40
Fagron	Vitamina E acetato pó 50%	022402A012	BR20043	40
Euro OTC	Concentrado seco de aceta…	2111015	25889SI	10
Euro OTC	Concentrado seco de aceta…	2207013	26279SI	20
Euro OTC	Concentrado seco de aceta…	2309007	26929SI	20
Fagron	Vitamina E acetato pó 50%	022403A011	BR20041SI	20
Fagron	Vitamina E acetato pó 50%	022402A012	BR20043SI	20

- 201 574 spectra from a total of 4035 batches from further 841 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 44 spectra from 15 *Apo-Ident* customers from 25 batches from the substance/substance group *Concentrado seco de acetato de alfa-tocoferol*.

- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bombastus	Concentrado seco de aceta…	1507001-02	1
Caelo	Concentrado seco de aceta…	1603046-02	2
Caelo	Concentrado seco de aceta…	1705003-01	1
EuRho	Concentrado seco de aceta…	1810024-01	1
Euro OTC	Concentrado seco de aceta…	1110021-02	2
Euro OTC	Concentrado seco de aceta…	1507001-01	2
Euro OTC	Concentrado seco de aceta…	160304602	1
Euro OTC	Concentrado seco de aceta…	1603046-02	1
Euro OTC	Concentrado seco de aceta…	170500301	1
Euro OTC	Concentrado seco de aceta…	1705003-01	1
Euro OTC	Concentrado seco de aceta…	1705003-02	1
Euro OTC	Concentrado seco de aceta…	1705003-04	2
Euro OTC	Concentrado seco de aceta…	1705003-05	1
Euro OTC	Concentrado seco de aceta…	181002401	1
Euro OTC	Concentrado seco de aceta…	1810024-01	4
Euro OTC	Concentrado seco de aceta…	190033-01	1
Euro OTC	Concentrado seco de aceta…	1907033-01	1
Euro OTC	Concentrado seco de aceta…	190703302	1
Euro OTC	Concentrado seco de aceta…	1907033-02	1
Euro OTC	Concentrado seco de aceta…	200502201	1
Euro OTC	Concentrado seco de aceta…	2005022-01	6
Euro OTC	Concentrado seco de aceta…	2106013-01	2
Euro OTC	Concentrado seco de aceta…	2111015-01	1
Euro OTC	Concentrado seco de aceta…	2207013-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Sanacorp	Concentrado seco de aceta…	150700101	1
Fagron	Concentrado seco de aceta…	13H30-B02-287169	1
Fagron	Concentrado seco de aceta…	16H30-B05-326792	1
Kehr	Concentrado seco de aceta…	1705003-03	2
Sanacorp	Concentrado seco de aceta…	1705003-03	1

- 236 023 spectra from 1515 *Apo-Ident* customers from a total of 49 234 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Concentrado seco de acetato de alfa-tocoferol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Concentrado seco de acetato de alfa-tocoferol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	500	0	152 462
Type B	0	468	42	201 574
Type C	0	44	0	236 023

The substance/substance group *Concentrado seco de acetato de alfa-tocoferol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8000 %)
Type B	100.0000 % (> 99.9912 %)	91.7647 % (> 91.1765 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.3636 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20907	21680	7,03	116,28
21609	21609	0,00	116,63
21680	21680	0,00	119,79
21842	21842	0,00	118,52
21959	21680	11,27	131,82
22543	22543	0,00	123,37
24841	24841	0,00	144,83
25277	25277	0,00	126,67
25599	25599	0,00	136,21
BR20042	BR20042	0,00	83,15

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cromoglicato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20775-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cromoglicato de sódio; Natrii cromoglicas

Special notes

When selecting the *Cromoglicato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cromoglicato de sódio	11	12	14

Second-stage model

For differentiation of the substance/substance group *Cromoglicato de sódio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cromoglicato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	97,55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cromoglicato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cromoglicato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cromoglicato de sódio	11114501	20776	80	20110518
Caelo	Cromoglicato de sódio	13232802	21375	20	1505352
Caelo	Cromoglicato de sódio	13232802	21376	110	20130905
Caelo	Cromoglicato de sódio	15224404	21990	60	20150625
Caelo	Cromoglicato de sódio	20003498	25641	40	20201120*
Euro OTC	Cromoglicato de sódio	1403017-01	21981	60	20140505
Euro OTC	Cromoglicato de sódio	1510018	22231	60	20151109*
Euro OTC	Cromoglicato de sódio	1703027	23383	40	20170405*
Euro OTC	Cromoglicato de sódio	2012005	25570	40	20210115*
Euro OTC	Cromoglicato de sódio	2407017	27366	40	20240814*
Fagron	Cromoglicato de sódio	12C09-N02	20775	79	1401553
Fagron	Cromoglicato de sódio	13G24-N04	21260	40	20130515

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 669 spectra of 12 reference samples from the substance/substance group *Cromoglicato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 293 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 530 spectra of 15 reference samples from the substance/substance group *Cromoglicato de sódio*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cromoglicato de sódio	173081	23855	30
Caelo	Cromoglicato de sódio	182657	24382	40
Euro OTC	Cromoglicato de sódio	1112003-01	20778	40
Euro OTC	Cromoglicato de sódio	1711024	23871	40
Euro OTC	Cromoglicato de sódio	1811016	24424	40
Euro OTC	Cromoglicato de sódio	2004037	25268	40
Euro OTC	Cromoglicato de sódio	2007031	25454	40
Euro OTC	Cromoglicato de sódio	2211013	26432	40
Euro OTC	Cromoglicato de sódio	2306002	26767	40
Euro OTC	Cromoglicato de sódio	2306008	26768	40
Fagron	Cromoglicato de sódio	15C23-B01-307751	22972	40
Fagron	Cromoglicato de sódio	23A04-B02-224458	26608	40
Euro OTC	Cromoglicato de sódio	2211013	26432SI	20
Euro OTC	Cromoglicato de sódio	2306002	26767SI	20
Fagron	Cromoglicato de sódio	23A04-B02-224458	26608SI	20

- 201 554 spectra from a total of 4033 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 19 *Apo-Ident* customers from 17 batches from the substance/substance group *Cromoglicato de sódio*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bombastus	Cromoglicato de sódio	15414502	1
Caelo	Cromoglicato de sódio	12301102	1
Caelo	Cromoglicato de sódio	15224404	1
Caelo	Cromoglicato de sódio	16270705	3
Caelo	Cromoglicato de sódio	17308104	1
Caelo	Cromoglicato de sódio	18265706	5
Caelo	Cromoglicato de sódio	18265707	1
Caelo	Cromoglicato de sódio	20003498009	1
Caelo	Cromoglicato de sódio	20003499001	2
Caelo	Cromoglicato de sódio	5113A-02831	1
Caesar & Loretz GmbH...	Cromoglicato de sódio	18265704	2
E Plus	Cromoglicato de sódio	15414502	1
Euro OTC	Cromoglicato de sódio	1403017-01	1
Euro OTC	Cromoglicato de sódio	1510018-01	1
Euro OTC	Cromoglicato de sódio	170302701	1
Euro OTC	Cromoglicato de sódio	1850002692	1
Fagron	Cromoglicato de sódio	13E22-N11	1
Fagron	Cromoglicato de sódio	13G24-N04	1
Sanacorp	Cromoglicato de sódio	20003499001	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cromoglicato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cromoglicato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	668	1	152 293
Type B	0	530	0	201 554
Type C	0	27	0	236 040

The substance/substance group *Cromoglicato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	99.8505 % (> 99.4021 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8679 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20775	20775	0,00	235,87
20776	22231	42,22	237,96
21260	22231	15,10	229,93
21375	21375	0,00	299,04
21376	21375	22,94	254,71
21981	22231	26,22	203,86
21990	22231	23,06	219,84
22231	22231	0,00	219,18
23383	23383	0,00	216,57
25570	25570	0,00	225,26
25641	25641	0,00	225,96
27366	27366	0,00	320,99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Curcumina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006686-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Curcumina

Special notes

When selecting the *Curcumina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Curcumina	2	1	0

Second-stage model

For differentiation of the substance/substance group *Curcumina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Curcumina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	122,60	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Curcumina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Curcumina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Curcumina	CP2404071	BR20026	40	20240410*
Fagron	Curcumina	CP2403046	BR20028	40	20240320*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Curcumina*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 4 reference samples from the substance/substance group *Curcumina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Curcumina	CP2403043	BR20027	40
Fagron	Curcumina	CP2404071	BR20026SI†	20
Fagron	Curcumina	CP2403043	BR20027SI	20
Fagron	Curcumina	CP2403046	BR20028SI†	20

- 201 984 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Curcumina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Curcumina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

relevant spectra of the various substances were compared with *Curcumina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	100	0	201 984
Type C	0	0	0	236 067

The substance/substance group *Curcumina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
BR20026	BR20026	0,00	255,59
BR20028	BR20028	0,00	265,30

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dexametasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20009-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dexametasona; Dexamethasonum

Special notes

When selecting the *Dexametasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dexametasona	10	17	387

Second-stage model

For differentiation of the substance/substance group *Dexametasona* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dexametasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	67,36	–
⋮	⋮	⋮
Betametasona	>50	34,36
Prednisolona	>50	39,87
Fluocinolona acetonida	>50	51,18
Triancinolona acetonido	>50	57,26
Metilprednisolona	>50	68,95
Tirotricina	>50	135,68
Gramicidina	>50	184,52

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dexametasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dexametasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dexametasona	13084315	21403	60	AR-15-FG-006810-01
Caelo	Dexametasona	15054627	23169	40	20150420
Caelo	Dexametasona	190221	24504	40	20190214*
Caelo	Dexametasona	190221	24504SI	40	20190214*
Caelo	Dexametasona	23002226	26967	40	20230922*
Euro OTC	Dexametasona	1303007-01	21289	40	1407432
Euro OTC	Dexametasona	1303007-01	21850	60	20130328
Euro OTC	Dexametasona	1601052	22364	45	20160225*
Euro OTC	Dexametasona	1601052	22364SI	45	20160225*
Euro OTC	Dexametasona	1611001	22914	40	20161212*
Euro OTC	Dexametasona	1611001	22914SI	37	20161212*
Euro OTC	Dexametasona	2005024	25301	40	20200824*
Fagron	Dexametasona	16F02-B05-324844	23168	40	20160711
Fagron	Dexametasona	19A24-B01-361445	24705	40	20190403

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 607 spectra of 14 reference samples from the substance/substance group *Dexametasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 355 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1518 spectra of 38 reference samples from the substance/substance group *Dexametasona*.
- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexametasona	13084306	21062	60
Caelo	Dexametasona	171042	23331	40
Caelo	Dexametasona	172856	23841	40
Caelo	Dexametasona	190865	24742	40
Caelo	Dexametasona	20002251	25633	40
Caelo	Dexametasona	21001380	25795	40
Caelo	Dexametasona	22000049	25996	40
Caelo	Dexametasona	22002762	26476	40
Euro OTC	Dexametasona	1209008-02	21078	60
Euro OTC	Dexametasona	1708004	23692	40
Euro OTC	Dexametasona	1806023	24136	40
Euro OTC	Dexametasona	1909011	24839	40
Euro OTC	Dexametasona	1708004-02	24867	40
Euro OTC	Dexametasona	2109019	25874	50
Euro OTC	Dexametasona	2208005	26264	40
Fagron	Dexametasona	19A24-B01-359626	24573	40
Fagron	Dexametasona	22A17-B06-218167	26074	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexametasona	15054627	23169SI†	20
Caelo	Dexametasona	171042	23331SI	24
Caelo	Dexametasona	172856	23841SI	40
Caelo	Dexametasona	190865	24742SI	40
Caelo	Dexametasona	20002251	25633SI	40
Caelo	Dexametasona	21001380	25795SI	40
Caelo	Dexametasona	22000049	25996SI	40
Caelo	Dexametasona	22002762	26476SI	40
Caelo	Dexametasona	23002226	26967SI†	40
Euro OTC	Dexametasona	1303007-01	21850SI†	45
Euro OTC	Dexametasona	1708004	23692SI	26
Euro OTC	Dexametasona	1806023	24136SI	33
Euro OTC	Dexametasona	1909011	24839SI	40
Euro OTC	Dexametasona	1708004-02	24867SI	40
Euro OTC	Dexametasona	2005024	25301SI†	40
Euro OTC	Dexametasona	2109019	25874SI	50
Euro OTC	Dexametasona	2208005	26264SI	40
Fagron	Dexametasona	16F02-B05-324844	23168SI†	30
Fagron	Dexametasona	19A24-B01-359626	24573SI	40
Fagron	Dexametasona	19A24-B01-361445	24705SI†	40
Fagron	Dexametasona	22A17-B06-218167	26074SI	40

- 200 566 spectra from a total of 4022 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2898 spectra from 954 *Apo-Ident* customers from 400 batches from the substance/substance group *Dexametasona*.

- Among them are spectra of independent samples from 386 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dexametasona	2005024-03	1
	Dexametasona	2109019	1
	Dexametasona	2109019-01	2
	Dexametasona	2109019-03	4
	Dexametasona	22000049004	1
	Dexametasona	22000049005	3
	Dexametasona	22000049009	2
	Dexametasona	22000049011	2
	Dexametasona	2200043005	1
	Dexametasona	2200276005	1
	Dexametasona	22002762003	5
	Dexametasona	22002762004	3
	Dexametasona	22002762005	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Dexametasona	22002762008	8
	Dexametasona	22002762009	5
	Dexametasona	22002762010	2
	Dexametasona	22002762011	2
	Dexametasona	22002762014	2
	Dexametasona	22002762015	7
	Dexametasona	22002762016	8
	Dexametasona	22002762017	2
	Dexametasona	2202762005	1
	Dexametasona	2202762017	1
	Dexametasona	2208005-01	10
	Dexametasona	2208005-02	1
	Dexametasona	2208005-03	1
	Dexametasona	22B26-B06-222195	2
	Dexametasona	23B23-B03220800	1
	Dexametasona	23B-23-B03-220800	1
07.2021	Dexametasona	1909011	1
AHC	Dexametasona	22002762016	1
AHD	Dexametasona	17104210	1
AHD	Dexametasona	17104211	1
AHD	Dexametasona	17L19-B03-344099	1
AHD	Dexametasona	1806023-01	1
AHD	Dexametasona	19022108	1
AHD	Dexametasona	1909011-01	1
AHD	Dexametasona	21001380002	1
AHD	Dexametasona	22002762008	1
AHD	Dexametasona	22002762015	1
AHD	Dexametasona	2208005-01	1
ALH	Dexametasona	15054617	2
Alliance Healthcare	Dexametasona	20003905004	1
Alliance/Caeolo	Dexametasona	19086503	1
Alliance/EuRho	Dexametasona	1909011-02	1
Alliance	Dexametasona	22002762005	1
alliance	Dexametasona	22002762008	1
Alliance	Dexametasona	22002762016	1
Anzag	Dexametasona	1233305	1
Anzag	Dexametasona	17332404	1
Anzag	Dexametasona	2200004909	1
Anzag	Dexametasona	22002762005	1
Apo ident	Dexametasona	1909011-02	2
Apo ident	Dexametasona	2005024-03	1
apomix	Dexametasona	1611001-01	1
Bombastus	Dexametasona	150546629	1
Bombastus	Dexametasona	17332418	1
Bombastus	Dexametasona	1806023-01	1
BUFA	Dexametasona	97A29FP-101103	2
Cael / GEHE	Dexametasona	19086513	1
Caelo	Dexametasona		3
Caelo	Dexametasona	10369920	8
Caelo	Dexametasona	10369921	2
Caelo	Dexametasona	11105502	1
Caelo	Dexametasona	111055-02	1
Caelo	Dexametasona	117019022107	1
Caelo	Dexametasona	117117332419	1
Caelo	Dexametasona	1203304788	1
Caelo	Dexametasona	12033301	3
Caelo	Dexametasona	12033303	1
Caelo	Dexametasona	12033304	1
Caelo	Dexametasona	12033305	4
Caelo	Dexametasona	12033307	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexametasona	12033308	2
Caelo	Dexametasona	12033312	2
Caelo	Dexametasona	12033314	7
Caelo	Dexametasona	12033315	4
Caelo	Dexametasona	12033317	5
Caelo	Dexametasona	12033318	4
Caelo	Dexametasona	1209008-01	1
Caelo	Dexametasona	12091306	1
Caelo	Dexametasona	12165803	1
Caelo	Dexametasona	12165804	1
Caelo	Dexametasona	1303007-03	1
Caelo	Dexametasona	13084304	2
Caelo	Dexametasona	13084305	5
Caelo	Dexametasona	13084306	3
Caelo	Dexametasona	13084307	2
Caelo	Dexametasona	13084308	2
Caelo	Dexametasona	13084309	1
Caelo	Dexametasona	13084310	8
Caelo	Dexametasona	13084313	4
Caelo	Dexametasona	13084316	4
Caelo	Dexametasona	13084317	7
Caelo	Dexametasona	13084319	5
Caelo	Dexametasona	13084320	2
Caelo	Dexametasona	130854306	1
Caelo	Dexametasona	13342310	1
Caelo	Dexametasona	1335213	1
Caelo	Dexametasona	13352302	9
Caelo	Dexametasona	13352303	1
Caelo	Dexametasona	13352304	1
Caelo	Dexametasona	13352308	7
Caelo	Dexametasona	13352309	2
Caelo	Dexametasona	13352310	17
Caelo	Dexametasona	13352311	1
Caelo	Dexametasona	13352312	15
Caelo	Dexametasona	13352315	2
Caelo	Dexametasona	13D12-N09	1
Caelo	Dexametasona	13G08-N13	2
Caelo	Dexametasona	14196402	3
Caelo	Dexametasona	1504610	1
Caelo	Dexametasona	1504618	1
Caelo	Dexametasona	1504631	1
Caelo	Dexametasona	15054506	1
Caelo	Dexametasona	15054602	7
Caelo	Dexametasona	15054603	3
Caelo	Dexametasona	15054605	11
Caelo	Dexametasona	15054606	14
Caelo	Dexametasona	15054609	5
Caelo	Dexametasona	15054610	1
Caelo	Dexametasona	15054611	7
Caelo	Dexametasona	15054614	5
Caelo	Dexametasona	15054616	6
Caelo	Dexametasona	15054617	11
Caelo	Dexametasona	15054618	3
Caelo	Dexametasona	15054620/170314D	1
Caelo	Dexametasona	15054621	9
Caelo	Dexametasona	15054622	35
Caelo	Dexametasona	15054623	10
Caelo	Dexametasona	15054627	2
Caelo	Dexametasona	15054628	11
Caelo	Dexametasona	15054629	20

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexametasona	15054631	6
Caelo	Dexametasona	1505623	1
Caelo	Dexametasona	15215601	1
Caelo	Dexametasona	15A05-B01-304637	1
Caelo	Dexametasona	15I04-B04-315528	1
Caelo	Dexametasona	15K17-B07-321457	1
Caelo	Dexametasona	1601052-01	1
Caelo	Dexametasona	1601052-02	3
Caelo	Dexametasona	16012207	1
Caelo	Dexametasona	160821D	1
Caelo	Dexametasona	161001-01	1
Caelo	Dexametasona	1611001-01	3
Caelo	Dexametasona	16K24-B05-330281	1
Caelo	Dexametasona	1704203	1
Caelo	Dexametasona	1704204	1
Caelo	Dexametasona	1708004-01	10
Caelo	Dexametasona	17081716	1
Caelo	Dexametasona	1708804-01	1
Caelo	Dexametasona	17104201	1
Caelo	Dexametasona	17104202	2
Caelo	Dexametasona	17104203	6
Caelo	Dexametasona	17104204	9
Caelo	Dexametasona	17104205	8
Caelo	Dexametasona	17104210	24
Caelo	Dexametasona	17104211	30
Caelo	Dexametasona	17104212	2
Caelo	Dexametasona	17104216	12
Caelo	Dexametasona	171042165511	1
Caelo	Dexametasona	171042165585	1
Caelo	Dexametasona	1714203	1
Caelo	Dexametasona	173322402	1
Caelo	Dexametasona	17332402	14
Caelo	Dexametasona	17332403	37
Caelo	Dexametasona	17332404	15
Caelo	Dexametasona	17332406	8
Caelo	Dexametasona	17332407	6
Caelo	Dexametasona	17332408	19
Caelo	Dexametasona	17332411	3
Caelo	Dexametasona	17332412	10
Caelo	Dexametasona	17332413	8
Caelo	Dexametasona	17332414	8
Caelo	Dexametasona	17332415	8
Caelo	Dexametasona	17332415-D20180115Ma	1
Caelo	Dexametasona	17332416	4
Caelo	Dexametasona	17332417	3
Caelo	Dexametasona	17332418	3
Caelo	Dexametasona	17332419	26
Caelo	Dexametasona	17e31-b01-338016	1
Caelo	Dexametasona	1806023-01	2
Caelo	Dexametasona	18121709	1
Caelo	Dexametasona	190022101	1
Caelo	Dexametasona	1902210	1
Caelo	Dexametasona	19022101	54
Caelo	Dexametasona	19022102	3
Caelo	Dexametasona	19022103	9
Caelo	Dexametasona	19022104	8
Caelo	Dexametasona	19022107	20
Caelo	Dexametasona	190221070	1
Caelo	Dexametasona	19022108	5
Caelo	Dexametasona	19022109	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexametasona	19022112	6
Caelo	Dexametasona	190222112	1
Caelo	Dexametasona	19056503	1
Caelo	Dexametasona	190865001	16
Caelo	Dexametasona	190865005	1
Caelo	Dexametasona	19086501	7
Caelo	Dexametasona	19086502	28
Caelo	Dexametasona	19086503	53
Caelo	Dexametasona	19086504	19
Caelo	Dexametasona	19086508	6
Caelo	Dexametasona	19086513	29
Caelo	Dexametasona	190901101	1
Caelo	Dexametasona	1909011-01	1
Caelo	Dexametasona	19096503	1
Caelo	Dexametasona	191072709	1
Caelo	Dexametasona	192245004	1
Caelo	Dexametasona	192876001	39
Caelo	Dexametasona	192876002	1
Caelo	Dexametasona	192876004	32
Caelo	Dexametasona	192876005	24
Caelo	Dexametasona	192876008	2
Caelo	Dexametasona	192876009	14
Caelo	Dexametasona	200002251001	2
Caelo	Dexametasona	200002251002	1
Caelo	Dexametasona	200002551001	1
Caelo	Dexametasona	200003905003	1
Caelo	Dexametasona	20002251001	26
Caelo	Dexametasona	20002251002	11
Caelo	Dexametasona	200039005004	1
Caelo	Dexametasona	20003905001	3
Caelo	Dexametasona	20003905002	16
Caelo	Dexametasona	20003905003	19
Caelo	Dexametasona	20003905004	11
Caelo	Dexametasona	20003905005	21
Caelo	Dexametasona	2000395004	2
Caelo	Dexametasona	2005024-01	3
Caelo	Dexametasona	2005024-02	1
Caelo	Dexametasona	2005024-03	1
Caelo	Dexametasona	200529SM	1
Caelo	Dexametasona	21001380001	4
Caelo	Dexametasona	21001380002	26
Caelo	Dexametasona	21001380003	11
Caelo	Dexametasona	21001380004	16
Caelo	Dexametasona	21001380008	3
Caelo	Dexametasona	21001380009	11
Caelo	Dexametasona	21001380009I	1
Caelo	Dexametasona	21001380010	13
Caelo	Dexametasona	21001380011	7
Caelo	Dexametasona	2100138003	1
Caelo	Dexametasona	2100138009	3
Caelo	Dexametasona	2100138009x2	2
Caelo	Dexametasona	2109019-01	1
Caelo	Dexametasona	2109019-02	1
Caelo	Dexametasona	22000019003	1
Caelo	Dexametasona	22000049002	1
Caelo	Dexametasona	22000049003	12
Caelo	Dexametasona	22000049004	7
Caelo	Dexametasona	22000049005	6
Caelo	Dexametasona	22000049009	1
Caelo	Dexametasona	22000049010	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexametasona	22000049011	5
Caelo	Dexametasona	2200049003	1
Caelo	Dexametasona	2200049004	1
Caelo	Dexametasona	2200049009	1
Caelo	Dexametasona	22002762001	1
Caelo	Dexametasona	22002762002	1
Caelo	Dexametasona	22002762003	14
Caelo	Dexametasona	22002762004	5
Caelo	Dexametasona	22002762005	2
Caelo	Dexametasona	22002762008	2
Caelo	Dexametasona	22002762009	1
Caelo	Dexametasona	22002762010	1
Caelo	Dexametasona	22002762014	1
Caelo	Dexametasona	22002762017	2
Caelo	Dexametasona	2884	1
Caelo	Dexametasona	3084310	1
Caelo	Dexametasona	6(19086504)	1
Caelo	Dexametasona	9383631	1
Caesar & Loretz GmbH...	Dexametasona	22000049005	1
Caesar & Loretz GmbH...	Dexametasona	17104211	2
Caesar & Loretz GmbH...	Dexametasona	19022107	1
Caesar & Loretz GmbH...	Dexametasona	22002762004	1
Caesar & Loretz GmbH...	Dexametasona	17332416	1
Caesar & Loretz GmbH...	Dexametasona	17332419	2
Caesar & Loretz GmbH...	Dexametasona	19086513	1
Caesar & Loretz GmbH...	Dexametasona	10369922	1
Caesar & Loretz GmbH/ AHD	Dexametasona	192876005	1
Caesar & Loretz GmbH...	Dexametasona	20002251001	1
Caesar & Loretz GmbH...	Dexametasona	19022101	1
Caesar & Loretz GmbH...	Dexametasona	192876004	2
Caesar & Loretz GmbH...	Dexametasona	192876005	1
Caesar & Loretz GmbH...	Dexametasona	20002251002	1
Caesar & Loretz GmbH...	Dexametasona	21001380002	2
Caesar & Loretz GmbH...	Dexametasona	20003905004	1
Caesar & Loretz GmbH...	Dexametasona	20003905002	1
Caesar & Loretz GmbH...	Dexametasona	22002762004	1
Caesar & Loretz GmbH...	Dexametasona	21001380004	1
Caesar & Loretz GmbH/AHD	Dexametasona	19086502	1
Caesar & Loretz GmbH/AHD	Dexametasona	22000049005	1
Caesar & Loretz GmbH...	Dexametasona	19086504	1
Caesar & Loretz GmbH...	Dexametasona	19086513	1
Caesar & Loretz GmbH/GEHE	Dexametasona	19086508	1
Caesar & Loretz GmbH/GEHE	Dexametasona	192876004	2
Caesar & Loretz GmbH/Gehe	Dexametasona	20003905002	1
Caesar & Loretz GmbH/Gehe	Dexametasona	20003905003	1
Caesar & Loretz GmbH/GEHE	Dexametasona	20003905003	1
Caesar & Loretz GmbH/Gehe	Dexametasona	21001380009	1
Caesar & Loretz GmbH...	Dexametasona	19022103	1
Caesar & Loretz GmbH...	Dexametasona	192876005	1
Caesar & Loretz GmbH...	Dexametasona	20003905004	1
Caesar & Loretz GmbH...	Dexametasona	22000049004	1
Caesar & Loretz GmbH...	Dexametasona	22002762009	1
Caesar & Loretz GmbH/Gö	Dexametasona	192876004	1
Caesar & Loretz GmbH...	Dexametasona	21001380009	1
Caesar & Loretz GmbH...	Dexametasona	22000049005	1
Caesar & Loretz GmbH...	Dexametasona	1806023-02	1
Caesar & Loretz GmbH...	Dexametasona	19022103	1
Caesar & Loretz GmbH...	Dexametasona	192876004	1
Caesar & Loretz GmbH...	Dexametasona	20002251002	1
Caesar & Loretz GmbH...	Dexametasona	21001380002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Kehr	Dexametasona	20003905003	1
Caesar & Loretz GmbH/Kehr	Dexametasona	22000049003	1
Caesar & Loretz GmbH/Krie	Dexametasona	19086503	1
Caesar & Loretz GmbH...	Dexametasona	19086502	1
Caesar & Loretz GmbH...	Dexametasona	192876005	1
Caesar & Loretz GmbH...	Dexametasona	20003905003	1
Caesar & Loretz GmbH...	Dexametasona	19086503	1
Caesar & Loretz GmbH...	Dexametasona	192876009	1
Caesar & Loretz GmbH...	Dexametasona	20003905003	1
Caesar & Loretz GmbH...	Dexametasona	22000049011	1
Caesar & Loretz GmbH/Ph	Dexametasona	21001380010	1
Caesar & Loretz GmbH/Pho	Dexametasona	20003905003	1
Caesar & Loretz GmbH...	Dexametasona	20003905003	1
Caesar & Loretz GmbH...	Dexametasona	19022112	1
Caesar & Loretz GmbH...	Dexametasona	19086502	1
Caesar & Loretz GmbH...	Dexametasona	19086503	1
Caesar & Loretz GmbH...	Dexametasona	19086508	1
Caesar & Loretz GmbH...	Dexametasona	21001380002	1
Caesar & Loretz GmbH...	Dexametasona	21001380003	1
Caesar & Loretz GmbH...	Dexametasona	21001380004	2
Caesar & Loretz GmbH/Sa	Dexametasona	192876004	2
Caesar & Loretz GmbH...	Dexametasona	1909011-01	1
Caesar & Loretz GmbH...	Dexametasona	192876009	1
Caesar & Loretz GmbH...	Dexametasona	20002251002	1
Caesar & Loretz GmbH	Dexametasona	15054622	1
Caesar & Loretz GmbH	Dexametasona	161100102	1
Caesar & Loretz GmbH	Dexametasona	17332408	1
Caesar & Loretz GmbH	Dexametasona	17332414	1
Caesar & Loretz GmbH	Dexametasona	17332415	1
Caesar & Loretz GmbH	Dexametasona	17332419	1
Caesar & Loretz GmbH	Dexametasona	19022101	9
Caesar & Loretz GmbH	Dexametasona	19022103	1
Caesar & Loretz GmbH	Dexametasona	19022104	1
Caesar & Loretz GmbH	Dexametasona	19022107	7
Caesar & Loretz GmbH	Dexametasona	19022108	1
Caesar & Loretz GmbH	Dexametasona	190865001	2
Caesar & Loretz GmbH	Dexametasona	19086502	10
Caesar & Loretz GmbH	Dexametasona	19086503	6
Caesar & Loretz GmbH	Dexametasona	19086504	7
Caesar & Loretz GmbH	Dexametasona	19086513	3
Caesar & Loretz GmbH	Dexametasona	1909011-01	1
Caesar & Loretz GmbH	Dexametasona	192876001	11
Caesar & Loretz GmbH	Dexametasona	192876002	1
Caesar & Loretz GmbH	Dexametasona	192876004	12
Caesar & Loretz GmbH	Dexametasona	192876005	3
Caesar & Loretz GmbH	Dexametasona	192876008	1
Caesar & Loretz GmbH	Dexametasona	192876009	6
Caesar & Loretz GmbH	Dexametasona	20002251001	10
Caesar & Loretz GmbH	Dexametasona	20002251002	4
Caesar & Loretz GmbH	Dexametasona	20003905001	1
Caesar & Loretz GmbH	Dexametasona	20003905002	10
Caesar & Loretz GmbH	Dexametasona	20003905003	6
Caesar & Loretz GmbH	Dexametasona	20003905004	5
Caesar & Loretz GmbH	Dexametasona	20003905005	6
Caesar & Loretz GmbH	Dexametasona	21001380002	14
Caesar & Loretz GmbH	Dexametasona	21001380003	3
Caesar & Loretz GmbH	Dexametasona	21001380004	5
Caesar & Loretz GmbH	Dexametasona	21001380008	1
Caesar & Loretz GmbH	Dexametasona	21001380009	11
Caesar & Loretz GmbH	Dexametasona	21001380010	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Dexametasona	21001380011	3
Caesar & Loretz GmbH	Dexametasona	22000049003	1
Caesar & Loretz GmbH	Dexametasona	22000049004	2
Caesar & Loretz GmbH	Dexametasona	22000049005	4
Caesar & Loretz GmbH	Dexametasona	22000049009	3
Caesar & Loretz GmbH	Dexametasona	22000049010	1
Caesar & Loretz GmbH	Dexametasona	22000049011	2
Caesar & Loretz GmbH	Dexametasona	22002762004	4
Caesar & Loretz GmbH	Dexametasona	22002762005	3
Caesar & Loretz GmbH	Dexametasona	22002762009	1
Caesar & Loretz GmbH	Dexametasona	22002762014	1
Caesar & Loretz Hilden	Dexametasona	17332419	1
Caesar & Loretz Hilden	Dexametasona	19086503	1
Caesar & Loretz Hilden	Dexametasona	192876001	2
Caesar & Loretz Hilden	Dexametasona	20003905005	1
Caesar & Loretz/AHD	Dexametasona	19086503	1
Caesar & Loretz/Noweda	Dexametasona	13084319	1
Caesar & Loretz/Noweda	Dexametasona	20002251001	1
Caesar & Loretz	Dexametasona	21001380009	1
Caesar / Gehe	Dexametasona	17332403	1
Caesar& Loretz/Geile...	Dexametasona	19022104	1
caesar&loretz GmbH,P...	Dexametasona	15054622	3
Caesar&Loretz GmbH,P...	Dexametasona	15054606	2
Caesar&Loretz GmbH/Gehe	Dexametasona	19022101	2
Caesar&Loretz GmbH	Dexametasona	20002251002	1
Caesar&Loretz GmbH	Dexametasona	20003905005	1
Caesar&Loretz GmbH	Dexametasona	22000049003	1
Caesar/Gehe	Dexametasona	190865001	2
caesar	Dexametasona	15054617	1
Caleo / Phoenix	Dexametasona	20003905002	2
Caleo	Dexametasona	15054602	2
calo	Dexametasona	17332403	1
Cealo	Dexametasona	17332404	1
Ebert & Jacobi	Dexametasona	1303007-03	1
Ebert & Jacobi	Dexametasona	1611001-01	3
Ebert&Jacobi	Dexametasona	1601052-01	1
Ebert-Jacobi	Dexametasona	1611001-01	1
EuRho / Phoenix	Dexametasona	1303007-03	1
EuRho / Phoenix	Dexametasona	15054631	1
EuRho / Phönix	Dexametasona	2109019-01	1
EuRho Anzag	Dexametasona	1601052-02	1
EuRho Gehe	Dexametasona	1909011-02	1
EuRho/ Gehe	Dexametasona	1708004-01	1
EuRho/ Noweda	Dexametasona	2109019-02	1
EuRho/Gehe	Dexametasona	1806023-01	1
EuRho/Noweda	Dexametasona	17008004-01	1
EuRho/Noweda	Dexametasona	1806023-01	1
EuRho/Noweda	Dexametasona	1806023-03	1
EuRho/Noweda	Dexametasona	1909011-02	1
EuRho/Phoenix	Dexametasona	1909011-02	1
EuRho/Sanacorp	Dexametasona	2005024-02	1
EuRho	Dexametasona	1708004-01	1
EuRho	Dexametasona	1806023_04	1
EuRho	Dexametasona	1806023-01	1
EuRho	Dexametasona	1909011-01	1
EuRho	Dexametasona	1909011-02	2
eurho	Dexametasona	2005024-01	1
EuRho	Dexametasona	2005024-01	3
EuRho	Dexametasona	2005024-02	1
EuRho	Dexametasona	2005024-03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Dexametasona	2109019-01	1
EuRho	Dexametasona	NUD180601	1
Eurho-Pharma	Dexametasona	1909011-02	1
Euro OTC	Dexametasona		4
Euro OTC	Dexametasona	1107006-01	1
Euro OTC	Dexametasona	111105501	1
Euro OTC	Dexametasona	1111055-01	5
Euro OTC	Dexametasona	1111055-02	2
Euro OTC	Dexametasona	1200008-01	1
Euro OTC	Dexametasona	1203032-01	4
Euro OTC	Dexametasona	1203032-02	3
Euro OTC	Dexametasona	1209008-01	11
Euro OTC	Dexametasona	120900802	2
Euro OTC	Dexametasona	1209008-02	26
Euro OTC	Dexametasona	13030007	1
Euro OTC	Dexametasona	13030007-01	1
Euro OTC	Dexametasona	1303007	1
Euro OTC	Dexametasona	130300701	4
Euro OTC	Dexametasona	1303007-01	34
Euro OTC	Dexametasona	130300702	2
Euro OTC	Dexametasona	1303007-02	10
Euro OTC	Dexametasona	130300703	2
Euro OTC	Dexametasona	1303007-03	27
Euro OTC	Dexametasona	1303007-04	2
Euro OTC	Dexametasona	13352309	1
Euro OTC	Dexametasona	14D11-B01-294031	1
Euro OTC	Dexametasona	15054621	1
Euro OTC	Dexametasona	1512211327	1
Euro OTC	Dexametasona	160105201	2
Euro OTC	Dexametasona	1601052-01	27
Euro OTC	Dexametasona	160105202	1
Euro OTC	Dexametasona	1601052-02	37
Euro OTC	Dexametasona	1601052-21	1
Euro OTC	Dexametasona	1611001	2
Euro OTC	Dexametasona	161100101	5
Euro OTC	Dexametasona	1611001-01	58
Euro OTC	Dexametasona	1611001-02	2
Euro OTC	Dexametasona	161101-01	1
Euro OTC	Dexametasona	1702004-01	1
Euro OTC	Dexametasona	17080004-01	1
Euro OTC	Dexametasona	1708004	1
Euro OTC	Dexametasona	170800401	2
Euro OTC	Dexametasona	1708004-01	89
Euro OTC	Dexametasona	1708004-02	6
Euro OTC	Dexametasona	1708804-01	1
Euro OTC	Dexametasona	17104203	1
Euro OTC	Dexametasona	17104204	1
Euro OTC	Dexametasona	17104210	1
Euro OTC	Dexametasona	17104211	1
Euro OTC	Dexametasona	17332403	1
Euro OTC	Dexametasona	180208D/1611001-01	1
Euro OTC	Dexametasona	1806023	2
Euro OTC	Dexametasona	1806023_03	1
Euro OTC	Dexametasona	180602301	2
Euro OTC	Dexametasona	1806023-01	59
Euro OTC	Dexametasona	1806023-010	1
Euro OTC	Dexametasona	180602302	2
Euro OTC	Dexametasona	1806023-02	18
Euro OTC	Dexametasona	1806023-03	7
Euro OTC	Dexametasona	1806023-04	19

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Dexametasona	1806023-24	1
Euro OTC	Dexametasona	1806032-02	1
Euro OTC	Dexametasona	19022103	1
Euro OTC	Dexametasona	1905014-01	1
Euro OTC	Dexametasona	190701	1
Euro OTC	Dexametasona	19086503	1
Euro OTC	Dexametasona	1909011	3
Euro OTC	Dexametasona	190901101	2
Euro OTC	Dexametasona	1909011-01	46
Euro OTC	Dexametasona	190901102	1
Euro OTC	Dexametasona	1909011-02	33
Euro OTC	Dexametasona	1909011-02P200622-1	1
Euro OTC	Dexametasona	19909011-02	1
Euro OTC	Dexametasona	20005024-01	1
Euro OTC	Dexametasona	2002024-01	2
Euro OTC	Dexametasona	2005021-03	1
Euro OTC	Dexametasona	2005024	1
Euro OTC	Dexametasona	2005024_04	1
Euro OTC	Dexametasona	200502401	1
Euro OTC	Dexametasona	2005024-01	59
Euro OTC	Dexametasona	200502402	1
Euro OTC	Dexametasona	2005024-02	31
Euro OTC	Dexametasona	200502403	2
Euro OTC	Dexametasona	2005024-03	37
Euro OTC	Dexametasona	2005024-04	5
Euro OTC	Dexametasona	21001215017	1
Euro OTC	Dexametasona	21009019-01	1
Euro OTC	Dexametasona	2109012-01	1
Euro OTC	Dexametasona	210901901	1
Euro OTC	Dexametasona	2109019-01	32
Euro OTC	Dexametasona	2109019-02	11
Euro OTC	Dexametasona	2109019-03	6
Euro OTC	Dexametasona	2109019-0306	1
Euro OTC	Dexametasona	21090919-01	1
Euro OTC	Dexametasona	2208005-01	1
Euro OTC	Dexametasona	4914501	1
Euro OTC	Dexametasona	5213A1327	1
Euro OTC	Dexametasona	700107	3
Euro OTC	Dexametasona	DB003/0213	3
Euro OTC	Dexametasona	DZ11005K	1
Euro OTC	Dexametasona	L53613	1
Euro OTC	Dexametasona	T45290	2
Euro RHO/Jenne	Dexametasona	1909011-02	1
Euro Rho/Jenne	Dexametasona	2005024-03	1
Euro/ Gehe	Dexametasona	1909011-03	1
Euro/ Gehe	Dexametasona	19G25-B02-363757	1
Euro/ Sanacorp	Dexametasona	1601052-01	2
Euro/Gehe	Dexametasona	1611001-01	1
Euro/Gehe	Dexametasona	1708004-01	2
Euro/Noweda	Dexametasona	1806023-01	1
Euro/Sana	Dexametasona	2109019-01	1
EuRoh/Fiebig	Dexametasona	1806023-01	1
EuRoh/Gehe	Dexametasona	1806023	1
Fagron	Dexametasona	11D26-N10	3
Fagron	Dexametasona	11F30-N02	1
Fagron	Dexametasona	11L08-N01	4
Fagron	Dexametasona	1209008-01	1
Fagron	Dexametasona	12A24-B01-35964	1
Fagron	Dexametasona	12B06-N12	2
Fagron	Dexametasona	12D26-N09	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dexametasona	12H21-N11	2
Fagron	Dexametasona	1303007-03	1
Fagron	Dexametasona	13D12-N09	3
Fagron	Dexametasona	13D12-N19	1
Fagron	Dexametasona	13G08-N13	3
Fagron	Dexametasona	13L30-B34-289691	2
Fagron	Dexametasona	14A22-B03	2
Fagron	Dexametasona	14A22-B03-290700	1
Fagron	Dexametasona	14A22-B03-290701	1
Fagron	Dexametasona	14A22-B03-294030	1
Fagron	Dexametasona	14D11-B01-294031	2
Fagron	Dexametasona	14D11-B01-294032	1
Fagron	Dexametasona	15/04-B04-315528	1
Fagron	Dexametasona	15054603	1
Fagron	Dexametasona	15054614	1
Fagron	Dexametasona	15A05-B01	1
Fagron	Dexametasona	15A05-B01-034636	1
Fagron	Dexametasona	15a05-b01-304636	1
Fagron	Dexametasona	15A05-B01-304636	3
Fagron	Dexametasona	15a05-b01-304637	1
Fagron	Dexametasona	15A05-B01-304637	1
Fagron	Dexametasona	15C16-B07	1
Fagron	Dexametasona	15C16-B07-308252	1
Fagron	Dexametasona	15I04-B04-315528	2
Fagron	Dexametasona	15K17-B07-321457	3
Fagron	Dexametasona	16/06-B03-327323	1
Fagron	Dexametasona	1601052-01	1
Fagron	Dexametasona	16I06-B03-327323	3
Fagron	Dexametasona	16I06-B03-327488	3
Fagron	Dexametasona	16K24B05330281	1
Fagron	Dexametasona	16K24-B05-330281	1
Fagron	Dexametasona	1708004-01	2
Fagron	Dexametasona	17104203	1
Fagron	Dexametasona	17332414	1
Fagron	Dexametasona	17C13-B07-332461	5
Fagron	Dexametasona	17E31-B01-331860	1
Fagron	Dexametasona	17E31-B01-338016	1
Fagron	Dexametasona	17E31B01338017	1
Fagron	Dexametasona	17L19-B03	1
Fagron	Dexametasona	17L19-B03-344099	2
Fagron	Dexametasona	17L19B03-344100	1
Fagron	Dexametasona	17L19-B03-344100	2
Fagron	Dexametasona	17L19-B03-344396	1
Fagron	Dexametasona	18D09-B06	1
Fagron	Dexametasona	18D09-B06-348185	3
Fagron	Dexametasona	18E08-B05-350243	4
Fagron	Dexametasona	18H07-B00-355632	1
Fagron	Dexametasona	18H07-B02-355632	1
Fagron	Dexametasona	18H07-B02-356113	1
Fagron	Dexametasona	19A24B01	1
Fagron	Dexametasona	19A24-B01	1
Fagron	Dexametasona	19A24-B01-359624	4
Fagron	Dexametasona	19A24-B01-359625	1
Fagron	Dexametasona	19A24-B01-359626	3
Fagron	Dexametasona	19A24-B01-361445	1
Fagron	Dexametasona	19G25-B02-363751	3
Fagron	Dexametasona	19G25-B02-363755	1
Fagron	Dexametasona	2005024-01	1
Fagron	Dexametasona	20B04-F06-369866	2
Fagron	Dexametasona	20B04-F06-369867	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dexametasona	20E08-F04-370660	1
Fagron	Dexametasona	20F19-F08	1
Fagron	Dexametasona	20F19-F08-371577	4
Fagron	Dexametasona	20F19-F08-371578	1
Fagron	Dexametasona	20K05-F04-375225	2
Fagron	Dexametasona	21C11-F03-377848	4
Fagron	Dexametasona	21C11-F03-378501	5
Fagron	Dexametasona	21H13-B20-216247	1
Fagron	Dexametasona	22A17-B06-216246	5
Fagron	Dexametasona	22B26-B06-220498	1
Fagron	Dexametasona	2314A-01327	1
Fagron	Dexametasona	700107-0002	1
Fagron	Dexametasona	DZ11005K12B06-N12	1
Fagron	Dexametasona	F03-3778408	1
Fagron	Dexametasona	F06-3698606	2
Fagron	Dexametasona	NUD160702	1
Fagron	Dexametasona	NUD180601	1
Fargon/Noweda	Dexametasona	19A24-B01	2
Fiebig	Dexametasona	19086513	1
Fiebig	Dexametasona	20003905002	1
Gatt-Koller	Dexametasona	1801087	1
GEHE 12.03.2014	Dexametasona	13084306	1
Gehe 8.04.2014	Dexametasona	13084310	2
Gehe amax	Dexametasona	1806023-04	1
Gehe Rostock	Dexametasona	22002762004	1
Gehe, Tianyao pharma...	Dexametasona	1909011-01	1
Gehe/ Euro	Dexametasona	2005024-01	1
Gehe	Dexametasona	1203032-02	1
Gehe	Dexametasona	120900802	1
Gehe	Dexametasona	13084317	1
Gehe	Dexametasona	13D12-N09	2
Gehe	Dexametasona	15054602	2
Gehe	Dexametasona	15054621	1
Gehe	Dexametasona	15054629	1
Gehe	Dexametasona	15054631	1
Gehe	Dexametasona	1601052-02	1
Gehe	Dexametasona	1708004-01	2
Gehe	Dexametasona	17104210	1
Gehe	Dexametasona	17104212	1
Gehe	Dexametasona	17332404	1
GEHE	Dexametasona	17L19-B03-344099	1
Gehe	Dexametasona	1806023-02	2
GEHE	Dexametasona	18H07-B02	1
Gehe	Dexametasona	19086501	1
Gehe	Dexametasona	192876004	1
Gehe	Dexametasona	20003905003	1
Gehe	Dexametasona	2005024-01	1
Gehe	Dexametasona	2005024-04	1
Gehe	Dexametasona	2200004901	1
gehe	Dexametasona	220800501	1
Gehe	Dexametasona	F03-3785001	1
Geibo	Dexametasona	22002762015	1
Geilenkirchen	Dexametasona	17104205	1
Henry Lamotte Oils GmbH	Dexametasona	13084304	1
Jenne	Dexametasona	1806023-01	1
Jenne	Dexametasona	1806023-02	1
Jenne	Dexametasona	1909011-01	1
Jenne	Dexametasona	20002251002	1
Jenne	Dexametasona	2005024-03	1
Jenne	Dexametasona	22002762008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Dexametasona	22002762016	2
Kehr/Fargon	Dexametasona	1806023-01	2
Kehr	Dexametasona	17104205	1
Kehr	Dexametasona	17104210	1
Kehr	Dexametasona	19086508	1
Kehr	Dexametasona	2109019-03	1
Kehr	Dexametasona	22002762004	1
Krieger	Dexametasona	17332406	1
L10	Dexametasona	1708004-01	1
Noweda 02.12.2019	Dexametasona	1806023-04	1
Noweda Taucha	Dexametasona	2109019-01	2
Noweda	Dexametasona	12033307	2
Noweda	Dexametasona	1303007-03	1
Noweda	Dexametasona	1708004-01	1
Noweda	Dexametasona	1708004-02	1
Noweda	Dexametasona	17104204	1
Noweda	Dexametasona	1806023-01	1
Noweda	Dexametasona	1806023-04	1
Noweda	Dexametasona	19022101	2
Noweda	Dexametasona	19086503	1
Noweda	Dexametasona	1909011-01	1
Noweda	Dexametasona	20002251001	2
Noweda	Dexametasona	20003905002	1
Noweda	Dexametasona	200039050022003905003	1
Noweda	Dexametasona	20003905003	1
Noweda	Dexametasona	200502404	1
Noweda	Dexametasona	21001380003	1
Noweda	Dexametasona	2109019-03	1
Noweda	Dexametasona	22002762008	1
Noweda	Dexametasona	22002762010	1
Noweda	Dexametasona	22002762014	1
Noweda	Dexametasona	2208005-01	1
PH Euro 8,0	Dexametasona	15054610	1
Pharmacia / Gehe	Dexametasona	M62488	1
Pharmacia&Upjohn Comp	Dexametasona	1209008-02	1
Pharmacia&Upjohn Com...	Dexametasona	1601052-02	1
Phoenix Goettin	Dexametasona	117113352302	1
Phoenix	Dexametasona	10369928	1
Phoenix	Dexametasona	13084313	2
Phoenix	Dexametasona	13g08n13	1
Phoenix	Dexametasona	15I04-B04	1
Phoenix	Dexametasona	17332406	1
Phoenix	Dexametasona	17332416	1
Phoenix	Dexametasona	17332419	1
Phoenix	Dexametasona	19086503	1
Phoenix	Dexametasona	1909011-01	2
Phoenix	Dexametasona	20002251002	1
Phoenix	Dexametasona	20004529003	1
Phoenix	Dexametasona	200622506	1
Phoenix	Dexametasona	2109019-01	1
Phoenix	Dexametasona	22002762016	2
Phoenix	Dexametasona	3405	1
Phönix Euro 23.6.21	Dexametasona	2005024-03	1
Phönix Gotha	Dexametasona	12033315	1
Phönix Gotha	Dexametasona	13352311	1
Phönix Gotha	Dexametasona	17332408	1
Phönix	Dexametasona	12033314	1
PHÖNIX	Dexametasona	15K17-B07	1
Phönix	Dexametasona	1601052-02	3
Phönix	Dexametasona	1708004-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Dexametasona	1806023-01	1
Phönix	Dexametasona	19022101	1
Phönix	Dexametasona	1909011-01	1
Phönix	Dexametasona	1909011-02	1
Phönix	Dexametasona	192876005	1
Phönix	Dexametasona	2005024-03	1
PHönix	Dexametasona	2005024-03	1
phönix	Dexametasona	21001380009	1
Phönix	Dexametasona	22002762003	1
Phönix	Dexametasona	22002762010	1
Raben-Apotheke Mildenau	Dexametasona	1303007-01	2
Sanacorp	Dexametasona	13084308	1
Sanacorp	Dexametasona	13352309	1
Sanacorp	Dexametasona	1601052-01	1
Sanacorp	Dexametasona	17104211	1
Sanacorp	Dexametasona	17332402	1
Sanacorp	Dexametasona	2005024-01	1
Sanacorp	Dexametasona	21001380011	1
Sanacorp	Dexametasona	22002762004	1
Sanacorp	Dexametasona	22002762008	1
Sanacorp	Dexametasona	22002762009	1
Sanofi-Chimie FR/Noweda	Dexametasona	15054606	2
Sanofi-Chimie, FR/ Noweda	Dexametasona	12033308	1
Symbiotica/Noweda	Dexametasona	1601052-02	1
Symbiotica	Dexametasona	1303007-01	1
Symbiotica	Dexametasona	1303007-03	2
Symbiotika	Dexametasona	1303007-03	1
Tianjin Tianyao / Gehe	Dexametasona	17332408	1
Tianjin Tianyao Pharm/AHD	Dexametasona	1806023-01	1
Tianjin Tianyao Phar…	Dexametasona	200502404	1
Tianjin/Noweda	Dexametasona	NUD170802	1
Tianjin/Phoenix	Dexametasona	NUD190701	1
Tianjin/Phoenix	Dexametasona	NUD200402	1
unbekannt	Dexametasona	12D26-N09	1

- 233 169 spectra from 1515 *Apo-Ident* customers from a total of 48 867 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dexametasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dexametasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	607	0	152 355
Type B	0	1518	0	200 566
Type C	0	2837	61	233 169

The substance/substance group *Dexametasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0115 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6047 %)
Type C	100.0000 % (> 99.9007 %)	97.8951 % (> 97.7916 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21289	21289	0,00	170,00
21403	21403	0,00	98,20
21850	21289	16,64	170,69
22364	22364	0,00	86,51
22914	22914	0,00	91,41
23168	24504	9,73	174,49
23169	22364	7,15	86,84
24504	24504	0,00	175,60
24705	24504	9,25	174,09
25301	25301	0,00	175,93
26967	26967	0,00	177,14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diacetato de clorexidina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20989-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diacetato de clorexidina; Chlorhexidini acetas; Clorexidina, diacetato

Special notes

When selecting the *Diacetato de clorexidina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diacetato de clorexidina	11	6	137

Second-stage model

For differentiation of the substance/substance group *Diacetato de clorexidina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diacetato de clorexidina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	73,04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diacetato de clorexidina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diacetato de clorexidina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diacetato de clorexidina	12142726	20989	40	1402685
Caelo	Diacetato de clorexidina	12142727	21041	40	20120711
Caelo	Diacetato de clorexidina	154389	22456	60	20160309*
Caelo	Diacetato de clorexidina	15438914	22900	40	1704392
Caelo	Diacetato de clorexidina	15438914	22951	40	20160309
Caelo	Diacetato de clorexidina	15438913	23041	40	20160309*
Caelo	Diacetato de clorexidina	154389	23042	40	20160309*
Caelo	Diacetato de clorexidina	154389	23043	40	20160309*
Caelo	Diacetato de clorexidina	15438909	23044	40	20160309*
Caelo	Diacetato de clorexidina	154389	23048	40	20160309*
Caelo	Diacetato de clorexidina	22003198	26483	40	20221123*
Caelo	Diacetato de clorexidina	22003198	26483SI	40	20221123*
Fagron	Diacetato de clorexidina	14I08-B02-306223	22280	60	20140922
Fagron	Diacetato de clorexidina	14I08-B02-306223	22280SI	40	20140922
Fagron	Diacetato de clorexidina	15J02-B08-322916	22946	40	20151104
Fagron	Diacetato de clorexidina	15J02-B08-322916	22947	40	20151104
Fagron	Diacetato de clorexidina	22C12-B01-223585	26456	40	20220610
Fagron	Diacetato de clorexidina	22C12-B01-223585	26456SI	40	20220610
Fagron	Diacetato de clorexidina	23A26-B06-230994	26816	40	20230313
Fagron	Diacetato de clorexidina	23A26-B06-230994	26816SI	40	20230313

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 840 spectra of 20 reference samples from the substance/substance group *Diacetato de clorexidina*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 122 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 475 spectra of 12 reference samples from the substance/substance group *Diacetato de clorexidina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diacetato de clorexidina	152610	23045	40
Caelo	Diacetato de clorexidina	171858	23640	40
Caelo	Diacetato de clorexidina	21001181	25696	50
Caelo	Diacetato de clorexidina	22000764	26116	35
Caelo	Diacetato de clorexidina	23001289	26832	30
Fagron	Diacetato de clorexidina	18A17-B02-354548	25486	40
Caelo	Diacetato de clorexidina	15438914	22951SI†	40
Caelo	Diacetato de clorexidina	21001181	25696SI	50
Caelo	Diacetato de clorexidina	22000764	26116SI	40
Caelo	Diacetato de clorexidina	23001289	26832SI	30
Fagron	Diacetato de clorexidina	15J02-B08-322916	22947SI†	40
Fagron	Diacetato de clorexidina	18A17-B02-354548	25486SI	40

- 201 609 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1149 spectra from 626 *Apo-Ident* customers from 145 batches from the substance/substance group *Diacetato de clorexidina*.
- Among them are spectra of independent samples from 136 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Diacetato de clorexidina	19122104	1
	Diacetato de clorexidina	22003123004	1
	Diacetato de clorexidina	22003123005	2
	Diacetato de clorexidina	22003123009	14
	Diacetato de clorexidina	22003123010	5
	Diacetato de clorexidina	22003123017	14
	Diacetato de clorexidina	22C12-B01-223585	2
	Diacetato de clorexidina	23001289005	2
	Diacetato de clorexidina	23001289006	2
	Diacetato de clorexidina	23001289008	4
	Diacetato de clorexidina	2300129800	1
	Diacetato de clorexidina	23003317002	1
AEP	Diacetato de clorexidina	200004515004	1
AEP	Diacetato de clorexidina	20004515004	1
AHD	Diacetato de clorexidina	17185812	1
AHD	Diacetato de clorexidina	22003123017	1
AHD	Diacetato de clorexidina	23001289006	2
AHL	Diacetato de clorexidina	15438903	1
Alliance Healthcare	Diacetato de clorexidina	12177510	1
Alliance	Diacetato de clorexidina	22003123005	1
Anzag	Diacetato de clorexidina	12177505	1
Anzag	Diacetato de clorexidina	18072404	1
Anzag	Diacetato de clorexidina	70558377	1
Bomastus / Alliance ...	Diacetato de clorexidina	17185804	1
Caelo	Diacetato de clorexidina	10154407	1
Caelo	Diacetato de clorexidina	10154417	1
Caelo	Diacetato de clorexidina	10154421	1
Caelo	Diacetato de clorexidina	10154424	1
Caelo	Diacetato de clorexidina	10154429	1
Caelo	Diacetato de clorexidina	10154430	2
Caelo	Diacetato de clorexidina	1072015C	1
Caelo	Diacetato de clorexidina	11204401	3
Caelo	Diacetato de clorexidina	11204402	1
Caelo	Diacetato de clorexidina	11204405	1
Caelo	Diacetato de clorexidina	11204406	2
Caelo	Diacetato de clorexidina	11204407	1
Caelo	Diacetato de clorexidina	11204408	2
Caelo	Diacetato de clorexidina	12142702	2
Caelo	Diacetato de clorexidina	12142704	6
Caelo	Diacetato de clorexidina	12142704ok	1
Caelo	Diacetato de clorexidina	12142705	3
Caelo	Diacetato de clorexidina	12142709	1
Caelo	Diacetato de clorexidina	12142715	4

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diacetato de clorexidina	12142720	10
Caelo	Diacetato de clorexidina	12142725	6
Caelo	Diacetato de clorexidina	12142726	9
Caelo	Diacetato de clorexidina	12142727	10
Caelo	Diacetato de clorexidina	12142734	13
Caelo	Diacetato de clorexidina	12177502	1
Caelo	Diacetato de clorexidina	12177503	2
Caelo	Diacetato de clorexidina	12177504	1
Caelo	Diacetato de clorexidina	12177505	3
Caelo	Diacetato de clorexidina	12177510	8
Caelo	Diacetato de clorexidina	123456	1
Caelo	Diacetato de clorexidina	1242720	1
Caelo	Diacetato de clorexidina	1317021	1
Caelo	Diacetato de clorexidina	13177001	6
Caelo	Diacetato de clorexidina	13177002	12
Caelo	Diacetato de clorexidina	13177007	20
Caelo	Diacetato de clorexidina	13177008	4
Caelo	Diacetato de clorexidina	13177009	1
Caelo	Diacetato de clorexidina	13177021	15
Caelo	Diacetato de clorexidina	13177022	1
Caelo	Diacetato de clorexidina	13177024	7
Caelo	Diacetato de clorexidina	15261003	7
Caelo	Diacetato de clorexidina	15261004	2
Caelo	Diacetato de clorexidina	15261005	7
Caelo	Diacetato de clorexidina	15261007	19
Caelo	Diacetato de clorexidina	15261009	15
Caelo	Diacetato de clorexidina	15261011	1
Caelo	Diacetato de clorexidina	15261012	10
Caelo	Diacetato de clorexidina	15261014	27
Caelo	Diacetato de clorexidina	15438902	9
Caelo	Diacetato de clorexidina	15438903	11
Caelo	Diacetato de clorexidina	15438909	5
Caelo	Diacetato de clorexidina	15438911	18
Caelo	Diacetato de clorexidina	15438913	1
Caelo	Diacetato de clorexidina	15438914	7
Caelo	Diacetato de clorexidina	15438917	12
Caelo	Diacetato de clorexidina	1543909	1
Caelo	Diacetato de clorexidina	15J02-B08-322916	1
Caelo	Diacetato de clorexidina	160912CH	1
Caelo	Diacetato de clorexidina	17185802	3
Caelo	Diacetato de clorexidina	17185803	6
Caelo	Diacetato de clorexidina	17185804	29
Caelo	Diacetato de clorexidina	17185805	6
Caelo	Diacetato de clorexidina	17185807	22
Caelo	Diacetato de clorexidina	17185808	20
Caelo	Diacetato de clorexidina	17185810	29
Caelo	Diacetato de clorexidina	17185811	24
Caelo	Diacetato de clorexidina	17185812	24
Caelo	Diacetato de clorexidina	17188504	1
Caelo	Diacetato de clorexidina	17325801	8
Caelo	Diacetato de clorexidina	17325803	32
Caelo	Diacetato de clorexidina	17325808	13
Caelo	Diacetato de clorexidina	17325809	35
Caelo	Diacetato de clorexidina	17326809	1
Caelo	Diacetato de clorexidina	1735801	1
Caelo	Diacetato de clorexidina	1735803	1
Caelo	Diacetato de clorexidina	1735809	1
Caelo	Diacetato de clorexidina	1785808	1
Caelo	Diacetato de clorexidina	180130CA/17185804	1
Caelo	Diacetato de clorexidina	18072403	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diacetato de clorexidina	18072404	21
Caelo	Diacetato de clorexidina	1907502	1
Caelo	Diacetato de clorexidina	190975001	22
Caelo	Diacetato de clorexidina	19097501	17
Caelo	Diacetato de clorexidina	19097502	33
Caelo	Diacetato de clorexidina	19121804	1
Caelo	Diacetato de clorexidina	191221001	11
Caelo	Diacetato de clorexidina	191221004	6
Caelo	Diacetato de clorexidina	19122103	4
Caelo	Diacetato de clorexidina	19122104	37
Caelo	Diacetato de clorexidina	200004515003	1
Caelo	Diacetato de clorexidina	20004515003	11
Caelo	Diacetato de clorexidina	20004515004	35
Caelo	Diacetato de clorexidina	20004515005	1
Caelo	Diacetato de clorexidina	20004515006	14
Caelo	Diacetato de clorexidina	20004515007	7
Caelo	Diacetato de clorexidina	2004515006	1
Caelo	Diacetato de clorexidina	2195172	1
Caelo	Diacetato de clorexidina	2195195	1
Caelo	Diacetato de clorexidina	22003123004	10
Caelo	Diacetato de clorexidina	22003123005	10
Caelo	Diacetato de clorexidina	22003123006	1
Caelo	Diacetato de clorexidina	22003123009	5
Caelo	Diacetato de clorexidina	22003123010	3
Caelo	Diacetato de clorexidina	22003123017	1
Caelo	Diacetato de clorexidina	22C12-B01-223585	1
Caelo	Diacetato de clorexidina	23001289008	1
Caelo	Diacetato de clorexidina	23012015D	1
Caelo	Diacetato de clorexidina	31032014B	1
Caelo	Diacetato de clorexidina	433218072404	1
Caelo	Diacetato de clorexidina	70558377	1
Caelo	Diacetato de clorexidina	9(191221004)	1
Caelo	Diacetato de clorexidina	9113903	1
Caelo	Diacetato de clorexidina	9113904	2
Caelo	Diacetato de clorexidina	91139389	1
Caelo	Diacetato de clorexidina	AK31122020	1
Caeol/ Noweda	Diacetato de clorexidina	15438911	1
Caeol/Noweda	Diacetato de clorexidina	19097502	2
Caesar & Loretz GmbH...	Diacetato de clorexidina	18072404	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	19122104	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	15261012	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	18072403	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	220031263004	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	12142720	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	17185812	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123005	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	20004515003	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123009	2
Caesar & Loretz GmbH...	Diacetato de clorexidina	19097501	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	19122103	2
Caesar & Loretz GmbH...	Diacetato de clorexidina	19122104	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123008	1
Caesar & Loretz GmbH/AHD	Diacetato de clorexidina	22003123004	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123009	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	19122104	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	20004515004	1
Caesar & Loretz GmbH/Gehe	Diacetato de clorexidina	17185810	1
Caesar & Loretz GmbH/Gehe	Diacetato de clorexidina	18072404	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	20004515003	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123010	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Diacetato de clorexidina	19122104	1
Caesar & Loretz GmbH/Otto	Diacetato de clorexidina	19097502	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	20004515004	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123010	2
Caesar & Loretz GmbH...	Diacetato de clorexidina	190975001	3
Caesar & Loretz GmbH...	Diacetato de clorexidina	191221001	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	20004515004	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	22003123004	1
Caesar & Loretz GmbH...	Diacetato de clorexidina	19122104	1
Caesar & Loretz GmbH	Diacetato de clorexidina	17185802	1
Caesar & Loretz GmbH	Diacetato de clorexidina	17185812	2
Caesar & Loretz GmbH	Diacetato de clorexidina	17325808	5
Caesar & Loretz GmbH	Diacetato de clorexidina	17325809	2
Caesar & Loretz GmbH	Diacetato de clorexidina	18072403	1
Caesar & Loretz GmbH	Diacetato de clorexidina	18072404	7
Caesar & Loretz GmbH	Diacetato de clorexidina	190975001	2
Caesar & Loretz GmbH	Diacetato de clorexidina	19097501	3
Caesar & Loretz GmbH	Diacetato de clorexidina	19097502	8
Caesar & Loretz GmbH	Diacetato de clorexidina	191221001	11
Caesar & Loretz GmbH	Diacetato de clorexidina	191221004	1
Caesar & Loretz GmbH	Diacetato de clorexidina	19122103	1
Caesar & Loretz GmbH	Diacetato de clorexidina	19122104	10
Caesar & Loretz GmbH	Diacetato de clorexidina	20004515003	6
Caesar & Loretz GmbH	Diacetato de clorexidina	20004515004	10
Caesar & Loretz GmbH	Diacetato de clorexidina	20004515007	1
Caesar & Loretz GmbH	Diacetato de clorexidina	22003123004	2
Caesar & Loretz GmbH	Diacetato de clorexidina	22003123005	7
Caesar & Loretz GmbH	Diacetato de clorexidina	22003123009	7
Caesar & Loretz GmbH	Diacetato de clorexidina	22003123010	2
Caesar & Loretz GmbH	Diacetato de clorexidina	22003123017	2
Caesar & Loretz GmbH	Diacetato de clorexidina	2203123004	1
Caesar & Loretz/Geil...	Diacetato de clorexidina	19097502	1
Caesar&loretz,Anzag	Diacetato de clorexidina	12142704	1
caesar	Diacetato de clorexidina	15261014	1
Cealo/Phoenix	Diacetato de clorexidina	22003123005	1
Cealo	Diacetato de clorexidina	13177002	2
cealo	Diacetato de clorexidina	17185804	1
Cealo	Diacetato de clorexidina	17325803	1
Ceasar & Loretz GmbH	Diacetato de clorexidina	80104278	1
Cordes/Noweda	Diacetato de clorexidina	15438914	1
Euro OTC	Diacetato de clorexidina	10154430	1
Euro OTC	Diacetato de clorexidina	15261004	1
Euro OTC	Diacetato de clorexidina	17185810	3
Euro OTC	Diacetato de clorexidina	17325809	1
Euro OTC	Diacetato de clorexidina	1785805	1
Fagron	Diacetato de clorexidina	12E14-N11	1
Fagron	Diacetato de clorexidina	13177008	1
Fagron	Diacetato de clorexidina	13E03-B06	1
Fagron	Diacetato de clorexidina	13E03-B06-287926	2
Fagron	Diacetato de clorexidina	13E03-B06-287929	1
Fagron	Diacetato de clorexidina	15261009	1
Fagron	Diacetato de clorexidina	15438901	1
Fagron	Diacetato de clorexidina	15J02-B08	2
Fagron	Diacetato de clorexidina	15J02-B08-322916	2
Fagron	Diacetato de clorexidina	17185811	1
Fagron	Diacetato de clorexidina	17325801	1
Fagron	Diacetato de clorexidina	17D25-B04-339937	3
Fagron	Diacetato de clorexidina	1-8991-1-01-01	1
Fagron	Diacetato de clorexidina	19F27-B03-364809	1
Fagron	Diacetato de clorexidina	22C12-B01-223585	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diacetato de clorexidina	A-130037	1
Fagron	Diacetato de clorexidina	A-170073	1
Fiebig	Diacetato de clorexidina	15261014	1
Fiebig	Diacetato de clorexidina	17185807	1
Fiebig	Diacetato de clorexidina	17325803	1
GEHE	Diacetato de clorexidina	12142734	1
Gehe	Diacetato de clorexidina	15261007	1
Gehe	Diacetato de clorexidina	15261009	2
Gehe	Diacetato de clorexidina	15438909	1
Gehe	Diacetato de clorexidina	17185804	1
Gehe	Diacetato de clorexidina	17185805	1
Gehe	Diacetato de clorexidina	17325803	1
Gehe	Diacetato de clorexidina	22003123009	2
Gehe	Diacetato de clorexidina	22003123017	1
Jenne	Diacetato de clorexidina	17185808	1
Jenne	Diacetato de clorexidina	17185810	1
Jenne	Diacetato de clorexidina	22003123010	1
Kehr	Diacetato de clorexidina	22003123017	1
keine Angabe	Diacetato de clorexidina	11204402	2
Medichem S.A. ES/Noweda	Diacetato de clorexidina	13177007	1
Nachprüfung	Diacetato de clorexidina	2082019-9	1
Noweda	Diacetato de clorexidina	12142720	1
Noweda	Diacetato de clorexidina	12142727	1
Noweda	Diacetato de clorexidina	15438911	2
Noweda	Diacetato de clorexidina	17185804	1
Noweda	Diacetato de clorexidina	17185805	1
Noweda	Diacetato de clorexidina	17185808	1
Noweda	Diacetato de clorexidina	17185811	1
Noweda	Diacetato de clorexidina	17325808	2
Noweda	Diacetato de clorexidina	1785803	1
Noweda	Diacetato de clorexidina	19097501	1
Noweda	Diacetato de clorexidina	22003123009	2
Phoenix	Diacetato de clorexidina	11204408	1
Phoenix	Diacetato de clorexidina	12142726	1
Phoenix	Diacetato de clorexidina	12142734	1
Phoenix	Diacetato de clorexidina	13177002	1
Phoenix	Diacetato de clorexidina	15438917	1
Phoenix	Diacetato de clorexidina	191221000	1
phönix	Diacetato de clorexidina		1
phönix	Diacetato de clorexidina	15438911	1
Phönix	Diacetato de clorexidina	15438917	1
Phönix	Diacetato de clorexidina	15J02-B08-322916	1
Phönix	Diacetato de clorexidina	17185803	1
Phönix	Diacetato de clorexidina	17185804	1
Phönix	Diacetato de clorexidina	17325803	1
phönix	Diacetato de clorexidina	19122104	1
Phönix	Diacetato de clorexidina	22003123004	1
Phönix	Diacetato de clorexidina	22003123009	1
Phönix	Diacetato de clorexidina	9113916	2
Phönix	Diacetato de clorexidina	Retest09113916	1
Sanacorp 107	Diacetato de clorexidina	190975001	1
Sanacorp	Diacetato de clorexidina		1
Sanacorp	Diacetato de clorexidina	12142734	1
Sanacorp	Diacetato de clorexidina	17185804	1
Sanacorp	Diacetato de clorexidina	18072403	1
SANACORP	Diacetato de clorexidina	19097502	1
Sanacorp	Diacetato de clorexidina	191221004	1
Sanacorp	Diacetato de clorexidina	22003123009	1
Sanacorp	Diacetato de clorexidina	22003123017	1
Sanacorp	Diacetato de clorexidina	7/AKD6	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Shaanxi dasehng Phar…	Diacetato de clorexidina	19122104	1
Shaanxi Dasheng Phar…	Diacetato de clorexidina	17185807	1
Shaanxi/Phoenix	Diacetato de clorexidina	CAB-180103	1
Wepa/Wepa	Diacetato de clorexidina	15438902	1

- 234 918 spectra from 1515 *Apo-Ident* customers from a total of 49 115 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diacetato de clorexidina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diacetato de clorexidina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	840	0	152 122
Type B	0	475	0	201 609
Type C	0	1135	14	234 918

The substance/substance group *Diacetato de clorexidina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2857 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7368 %)
Type C	100.0000 % (> 99.9007 %)	98.7815 % (> 98.5205 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20989	20989	0,00	179,91
21041	20989	18,34	179,86

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22280	22456	5,53	184,08
22456	22456	0,00	181,39
22900	22900	0,00	183,51
22946	23044	5,97	182,14
22947	22456	5,77	181,23
22951	22900	6,07	183,61
23041	23041	0,00	183,30
23042	23042	0,00	183,68
23043	23043	0,00	184,10
23044	23044	0,00	183,33
23048	23048	0,00	182,48
26456	22456	5,31	183,62
26483	26483	0,00	180,99
26816	20989	51,57	177,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diclofenaco sódico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20022-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diclofenaco sódico; Diclofenacum natricum

Special notes

When selecting the *Diclofenaco sódico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diclofenaco sódico	7	8	182

Second-stage model

For differentiation of the substance/substance group *Diclofenaco sódico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diclofenaco sódico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	140,64	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diclofenaco sódico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diclofenaco sódico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diclofenaco sódico	12214219	20883	20	20120815
Caelo	Diclofenaco sódico	13214311	21467	60	20130826
Caelo	Diclofenaco sódico	13214311	21470	60	20130826
Caelo	Diclofenaco sódico	163492	23037	40	20170112*
Euro OTC	Diclofenaco sódico	1403013-01	21330	40	20140401
Euro OTC	Diclofenaco sódico	1607016	22694	40	20160808*
Fagron	Diclofenaco sódico	13E03-N02	20886	40	20130515
Fagron	Diclofenaco sódico	12L28-B05	21261	40	20130123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 340 spectra of 8 reference samples from the substance/substance group *Diclofenaco sódico*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 390 spectra of 11 reference samples from the substance/substance group *Diclofenaco sódico*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diclofenaco sódico	21000065	25860	50
Euro OTC	Diclofenaco sódico	1711026	23872	40
Euro OTC	Diclofenaco sódico	1904008	24618	40
Euro OTC	Diclofenaco sódico	2009027	25416	40
Euro OTC	Diclofenaco sódico	2307012	26857	30
Fagron	Diclofenaco sódico	15D14-B04-307452	21979	60
Fagron	Diclofenaco sódico	19L02-F02-367737	25176	40
Fagron	Diclofenaco sódico	22L20-B04-230962	27167	40
Caelo	Diclofenaco sódico	21000065	25860SI	10
Euro OTC	Diclofenaco sódico	2307012	26857SI	20
Fagron	Diclofenaco sódico	22L20-B04-230962	27167SI	20

- 201 694 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 735 spectra from 336 *Apo-Ident* customers from 189 batches from the substance/substance group *Diclofenaco sódico*.

- Among them are spectra of independent samples from 181 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Diclofenaco sódico	2009027	2
	Diclofenaco sódico	2009027-02	1
	Diclofenaco sódico	2009027-05	5
	Diclofenaco sódico	21I29-B06-221805	6
	Diclofenaco sódico	21I29-B06-213571	1
	Diclofenaco sódico	22L20-B04-230962	1
	Diclofenaco sódico	23000021007	1
	Diclofenaco sódico	2307012-01	1
	Diclofenaco sódico	8/0206A	1
	Diclofenaco sódico	80423750002	1
	Diclofenaco sódico	RDS/2108/0206A	2
	Diclofenaco sódico	RDS21080206A	1
AHD	Diclofenaco sódico	1503014-01	1
AHD	Diclofenaco sódico	15D14B04314450	1
Aliance Healthcare	Diclofenaco sódico	2009027-03	1
Amoli/Phoenix	Diclofenaco sódico	20J01-F09	1
Amoli/Phoenix	Diclofenaco sódico	RDS/1807/0134A	1
Amoli	Diclofenaco sódico	1503014-01	1
Bombastus	Diclofenaco sódico	1711026-01	1
Caeli/Alliance	Diclofenaco sódico	18202602	1
Caelo	Diclofenaco sódico	11091201	1
Caelo	Diclofenaco sódico	12214202	1
Caelo	Diclofenaco sódico	12214205	1
Caelo	Diclofenaco sódico	12214206	1
Caelo	Diclofenaco sódico	12214219	2
Caelo	Diclofenaco sódico	12L28-B05	1
Caelo	Diclofenaco sódico	13214303	2
Caelo	Diclofenaco sódico	13214304	1
Caelo	Diclofenaco sódico	13214308	4
Caelo	Diclofenaco sódico	13214309	3
Caelo	Diclofenaco sódico	13214311	8
Caelo	Diclofenaco sódico	13214312	2
Caelo	Diclofenaco sódico	13214316	1
Caelo	Diclofenaco sódico	13214317	5
Caelo	Diclofenaco sódico	13214318	4
Caelo	Diclofenaco sódico	140301301	1
Caelo	Diclofenaco sódico	1503014-01	1
Caelo	Diclofenaco sódico	15169604	7
Caelo	Diclofenaco sódico	15169609	2
Caelo	Diclofenaco sódico	15169613	2
Caelo	Diclofenaco sódico	15169615	1
Caelo	Diclofenaco sódico	15169617	1
Caelo	Diclofenaco sódico	15169675	1
Caelo	Diclofenaco sódico	15278501	1
Caelo	Diclofenaco sódico	15278502	2
Caelo	Diclofenaco sódico	15278505	2
Caelo	Diclofenaco sódico	15278506	3
Caelo	Diclofenaco sódico	15278507	1
Caelo	Diclofenaco sódico	15K23-B03-318519	2
Caelo	Diclofenaco sódico	15K23-B03-325753	2
Caelo	Diclofenaco sódico	15K23-B03-325753	1
Caelo	Diclofenaco sódico	16/29-B04-334699	1
Caelo	Diclofenaco sódico	1607016-03	1
Caelo	Diclofenaco sódico	16349207	3
Caelo	Diclofenaco sódico	16349208	1
Caelo	Diclofenaco sódico	1711026-01	1
Caelo	Diclofenaco sódico	1711026-02	1
Caelo	Diclofenaco sódico	1711026-03	1
Caelo	Diclofenaco sódico	17J19-B01-345397	1
Caelo	Diclofenaco sódico	17J19-B01-352716	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diclofenaco sódico	18039202	1
Caelo	Diclofenaco sódico	18039203	3
Caelo	Diclofenaco sódico	18039208	1
Caelo	Diclofenaco sódico	18039210	4
Caelo	Diclofenaco sódico	182026003	1
Caelo	Diclofenaco sódico	182026004	6
Caelo	Diclofenaco sódico	18202602	2
Caelo	Diclofenaco sódico	18202606	1
Caelo	Diclofenaco sódico	18202609	7
Caelo	Diclofenaco sódico	20003803001	3
Caelo	Diclofenaco sódico	20003803002	2
Caelo	Diclofenaco sódico	20003803004	2
Caelo	Diclofenaco sódico	2000383002	1
Caelo	Diclofenaco sódico	2100005012	1
Caelo	Diclofenaco sódico	21000065003	1
Caelo	Diclofenaco sódico	21000065004	2
Caelo	Diclofenaco sódico	21000065006	1
Caelo	Diclofenaco sódico	21000065009	2
Caelo	Diclofenaco sódico	2100006501	1
Caelo	Diclofenaco sódico	21000065012	4
Caelo	Diclofenaco sódico	21I29-B06-221805	1
Caelo	Diclofenaco sódico	5081501	1
Caesar & Loretz GmbH	Diclofenaco sódico	182026004	2
Caesar & Loretz GmbH	Diclofenaco sódico	18202601	1
Caesar & Loretz GmbH	Diclofenaco sódico	18202602	1
Caesar & Loretz GmbH	Diclofenaco sódico	18202606	1
Caesar & Loretz GmbH	Diclofenaco sódico	18202609	1
Caesar & Loretz GmbH	Diclofenaco sódico	20003803001	3
Caesar & Loretz GmbH	Diclofenaco sódico	20003803002	1
Caesar & Loretz GmbH	Diclofenaco sódico	20003803004	1
Caesar & Loretz GmbH	Diclofenaco sódico	21000065002	1
Caesar & Loretz GmbH	Diclofenaco sódico	21000065006	1
Caesar & Loretz GmbH	Diclofenaco sódico	21000065012	2
Caesar & Loretz GmbH	Diclofenaco sódico	21000065013	1
Caesar & Loretz GmbH	Diclofenaco sódico	21000065015	2
Cealo	Diclofenaco sódico	160701601	1
Euph/Sanacorp	Diclofenaco sódico	171102603	1
EuRho / Gehe	Diclofenaco sódico	2009027-02	2
EuRho /Gumo	Diclofenaco sódico	1711028-03	1
EuRho/Jenne	Diclofenaco sódico	1(1711026-03)	1
Eurho/Noweda	Diclofenaco sódico	2009027-02	1
EuRho/Sanacorp	Diclofenaco sódico	1711026-02	2
EuRho/Sanacorp	Diclofenaco sódico	1904008-02	1
EuRho/Sanacorp	Diclofenaco sódico	2009027-01	1
EuRho/Spangro	Diclofenaco sódico	1711026-02	2
EuRho	Diclofenaco sódico	1206026-02	1
EuRho	Diclofenaco sódico	1503014-01	1
EuRho	Diclofenaco sódico	2009027-02	1
Euro OTC	Diclofenaco sódico	11091404	1
Euro OTC	Diclofenaco sódico	1111040-01	2
Euro OTC	Diclofenaco sódico	12060250	1
Euro OTC	Diclofenaco sódico	1206026	1
Euro OTC	Diclofenaco sódico	1206026-01	7
Euro OTC	Diclofenaco sódico	1206026-02	3
Euro OTC	Diclofenaco sódico	12214220	1
Euro OTC	Diclofenaco sódico	13111203	1
Euro OTC	Diclofenaco sódico	140301301	1
Euro OTC	Diclofenaco sódico	1403013-01	5
Euro OTC	Diclofenaco sódico	1403013-02	7
Euro OTC	Diclofenaco sódico	1403013-03	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Diclofenaco sódico	1503014-01	14
Euro OTC	Diclofenaco sódico	1503014-02	6
Euro OTC	Diclofenaco sódico	15169606	1
Euro OTC	Diclofenaco sódico	15K23-B03-321673	1
Euro OTC	Diclofenaco sódico	16067016-03	1
Euro OTC	Diclofenaco sódico	1607016-01	33
Euro OTC	Diclofenaco sódico	1607016-02	17
Euro OTC	Diclofenaco sódico	1607016-03	29
Euro OTC	Diclofenaco sódico	1711023-03	1
Euro OTC	Diclofenaco sódico	1711026	2
Euro OTC	Diclofenaco sódico	1711026-01	17
Euro OTC	Diclofenaco sódico	171102602	2
Euro OTC	Diclofenaco sódico	1711026-02	17
Euro OTC	Diclofenaco sódico	171102603	3
Euro OTC	Diclofenaco sódico	1711026-03	41
Euro OTC	Diclofenaco sódico	1711026-1	1
Euro OTC	Diclofenaco sódico	17111026_01	1
Euro OTC	Diclofenaco sódico	17J19-B01-350960	2
Euro OTC	Diclofenaco sódico	1807016-01	1
Euro OTC	Diclofenaco sódico	1904008	2
Euro OTC	Diclofenaco sódico	190400801	3
Euro OTC	Diclofenaco sódico	1904008-01	15
Euro OTC	Diclofenaco sódico	1904008-02	30
Euro OTC	Diclofenaco sódico	1904008-1	1
Euro OTC	Diclofenaco sódico	194008-02	1
Euro OTC	Diclofenaco sódico	19404008-01	1
Euro OTC	Diclofenaco sódico	2009027	1
Euro OTC	Diclofenaco sódico	2009027-01	18
Euro OTC	Diclofenaco sódico	2009027-02	36
Euro OTC	Diclofenaco sódico	2009027-03	8
Euro OTC	Diclofenaco sódico	2009027-04	1
Euro OTC	Diclofenaco sódico	2009027-05	1
Euro OTC	Diclofenaco sódico	2091715	1
Euro OTC	Diclofenaco sódico	21031703	1
Euro OTC	Diclofenaco sódico	23051814	1
Euro OTC	Diclofenaco sódico	25041403	1
Euro OTC	Diclofenaco sódico	301180730-21	1
Euro OTC	Diclofenaco sódico	31101802	1
Euro OTC	Diclofenaco sódico	8051812	1
Euro OTC	Diclofenaco sódico	AP201218-03	1
Euro OTC	Diclofenaco sódico	AP210516-20	1
EURO/all	Diclofenaco sódico	135796	1
Euro/Anzag	Diclofenaco sódico	1607016-03	1
Euro/L10	Diclofenaco sódico	1711026031904008-01	1
EURO/Noweda	Diclofenaco sódico	140301301	1
Euro/Phönix	Diclofenaco sódico	1711026	1
Euro/Phönix	Diclofenaco sódico	2009027-02	1
Europharm/Otto	Diclofenaco sódico	135796	1
EurRho/ Anzag	Diclofenaco sódico	1403013-03	1
Fagron	Diclofenaco sódico		1
Fagron	Diclofenaco sódico	10031505	1
Fagron	Diclofenaco sódico	12L28-B05-289773	2
Fagron	Diclofenaco sódico	135796-0002	1
Fagron	Diclofenaco sódico	13E03-N02	1
Fagron	Diclofenaco sódico	14031411	1
Fagron	Diclofenaco sódico	14G17-B08-0159A	1
Fagron	Diclofenaco sódico	14G17B08297032	1
Fagron	Diclofenaco sódico	14G17-B08-297032	6
Fagron	Diclofenaco sódico	15D14-B04	1
Fagron	Diclofenaco sódico	15D14-B04-307452	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diclofenaco sódico	15D14-B04-314450	4
Fagron	Diclofenaco sódico	15D14-B04-315835	1
Fagron	Diclofenaco sódico	15K23-B03	1
Fagron	Diclofenaco sódico	15K23-B03-318519	2
Fagron	Diclofenaco sódico	15K23-B03-321673	6
Fagron	Diclofenaco sódico	15K23-B03-324025	6
Fagron	Diclofenaco sódico	15K23-B03-325753	5
Fagron	Diclofenaco sódico	15K23-B03-327802	5
Fagron	Diclofenaco sódico	16/29-B04-332372	1
Fagron	Diclofenaco sódico	1607016-03	3
Fagron	Diclofenaco sódico	16I29-B04	1
Fagron	Diclofenaco sódico	16I29-B04-332372	4
Fagron	Diclofenaco sódico	16l29	1
Fagron	Diclofenaco sódico	17F02	1
Fagron	Diclofenaco sódico	17F02-B05	1
Fagron	Diclofenaco sódico	17F02-B05-338797	8
Fagron	Diclofenaco sódico	17J19-B01	1
Fagron	Diclofenaco sódico	17j19-B01-342310	1
Fagron	Diclofenaco sódico	17J19-B01-342310	4
Fagron	Diclofenaco sódico	17J19-B01-345397	2
Fagron	Diclofenaco sódico	17J19-B01-350960	3
Fagron	Diclofenaco sódico	17J19-B01-352716	3
Fagron	Diclofenaco sódico	17j19-b01-354796	1
Fagron	Diclofenaco sódico	17j19-B01-354796	1
Fagron	Diclofenaco sódico	17J19-B01-354796	2
Fagron	Diclofenaco sódico	17J19-B01B350960	1
Fagron	Diclofenaco sódico	18H24-B07	2
Fagron	Diclofenaco sódico	18H24-B07-357416	5
Fagron	Diclofenaco sódico	18H24-B07-358891	5
Fagron	Diclofenaco sódico	19L02-F02	1
Fagron	Diclofenaco sódico	19L02-F02-367737	4
Fagron	Diclofenaco sódico	19L02-F02-368388	3
Fagron	Diclofenaco sódico	19L02-F02-369055	1
Fagron	Diclofenaco sódico	19LO2-FO2-367737	1
Fagron	Diclofenaco sódico	20J01-F09-0043A	1
Fagron	Diclofenaco sódico	20J01-F09-374507	6
Fagron	Diclofenaco sódico	21129-BO6-221805	1
Fagron	Diclofenaco sódico	21C26-F04-377842	3
Fagron	Diclofenaco sódico	21I29-B06-221805	5
Fagron	Diclofenaco sódico	314450	1
Fagron	Diclofenaco sódico	5041401	1
Fagron	Diclofenaco sódico	F02-3677307	1
Fagron	Diclofenaco sódico	F02-367737	1
Fagron	Diclofenaco sódico	F02-3683808	1
Fagron	Diclofenaco sódico	f04-3778402	1
Fagron	Diclofenaco sódico	F09-3745007	2
Fagron	Diclofenaco sódico	RDS/1405/0159A	1
Fagron	Diclofenaco sódico	RDS/1607/334699	1
Fargon GmbH & Co.KG	Diclofenaco sódico	15K23-B03-325753	1
Fargron	Diclofenaco sódico	14G17-B08-297032	1
FIEBIG	Diclofenaco sódico	20003803002	1
Fischar/Phönix	Diclofenaco sódico	13214311	1
Fragon/Sanacorp	Diclofenaco sódico	19L02-F02-3699055	1
Gehe	Diclofenaco sódico	1206026-01	1
Gehe	Diclofenaco sódico	15278502	1
Gehe	Diclofenaco sódico	1711026-03	1
GEHE	Diclofenaco sódico	17J19-B01-342310	1
Gehe	Diclofenaco sódico	1904008-01	2
Gehe	Diclofenaco sódico	547718202609	1
Gehe	Diclofenaco sódico	A22370D230	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Diclofenaco sódico	15278502	2
Hedinger/Phoenix	Diclofenaco sódico	15278506	3
Hubei Gedian Humanwe…	Diclofenaco sódico	1711026-02	1
JENNE	Diclofenaco sódico	17J19-B01	1
Kehr	Diclofenaco sódico	1711026-03	1
L11	Diclofenaco sódico	15278506	1
L12	Diclofenaco sódico	18039202	1
Noveda	Diclofenaco sódico	30120071252	1
Noweda/EuRho	Diclofenaco sódico	1904008-02	1
Noweda	Diclofenaco sódico	11G12-N06	1
Noweda	Diclofenaco sódico	1403013-01	1
Noweda	Diclofenaco sódico	15278504	1
Noweda	Diclofenaco sódico	1711026-03	1
Noweda	Diclofenaco sódico	18039202	1
Noweda	Diclofenaco sódico	18202602	1
Noweda	Diclofenaco sódico	1904008-01	1
Noweda	Diclofenaco sódico	19L02-F02-367737	1
Noweda	Diclofenaco sódico	2009027-03	1
NOWEDA	Diclofenaco sódico	2009027-05	1
Phoenix	Diclofenaco sódico	15K23-B03	1
Phoenix	Diclofenaco sódico	1711026-02	1
Phoenix	Diclofenaco sódico	19L02-F02-368388	1
Phönix	Diclofenaco sódico	1403013-03	1
Phönix	Diclofenaco sódico	1607016-02	1
Phönix	Diclofenaco sódico	1711026-03	1
PHÖNIX	Diclofenaco sódico	17F02-B05	1
Phönix	Diclofenaco sódico	17F02-B05-338797	1
Phönix	Diclofenaco sódico	21i29-b06-213571	1
Phönix	Diclofenaco sódico	F02-3677307	1
sana	Diclofenaco sódico	2009027-03	1
Sanacorp	Diclofenaco sódico	1206026-01	1
SANACORP	Diclofenaco sódico	18039204	1
SANACORP	Diclofenaco sódico	18202606	1
Sanacorp	Diclofenaco sódico	2009027-03	1
Sanacorp	Diclofenaco sódico	3616Q-02994	1
siehe Protokoll	Diclofenaco sódico	15169617	1

- 235 332 spectra from 1515 *Apo-Ident* customers from a total of 49 069 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diclofenaco sódico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diclofenaco sódico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	390	0	201 694
Type C	0	732	3	235 332

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Diclofenaco sódico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4615 %)
Type C	100.0000 % (> 99.9007 %)	99.5918 % (> 99.1837 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20883	23037	10,93	318,45
20886	23037	24,16	326,31
21261	23037	29,34	317,54
21330	23037	18,02	326,19
21467	23037	16,43	323,16
21470	23037	6,93	329,50
22694	22694	0,00	256,71
23037	23037	0,00	321,31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dicloridrato de histamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20963-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dicloridrato de histamina; Histamina, dicloridrato; Histamini dihydrochloridum

Special notes

When selecting the *Dicloridrato de histamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dicloridrato de histamina	6	6	31

Second-stage model

For differentiation of the substance/substance group *Dicloridrato de histamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dicloridrato de histamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	89,42	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dicloridrato de histamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dicloridrato de histamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Dicloridrato de histamina	1111004-02	20963	40	1403674
Euro OTC	Dicloridrato de histamina	1506030	21863	60	20150706*
Euro OTC	Dicloridrato de histamina	2004012	25166	40	20200525*
Euro OTC	Dicloridrato de histamina	2009009	25413	40	20201005*
Fagron	Dicloridrato de histamina	14G16-B02-299175	21668	100	20140729
Fagron	Dicloridrato de histamina	19D19-B02-361228	24589	40	20190516

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 6 reference samples from the substance/substance group *Dicloridrato de histamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 340 spectra of 10 reference samples from the substance/substance group *Dicloridrato de histamina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Dicloridrato de histamina	1812018	24541	40
Euro OTC	Dicloridrato de histamina	1905003	24616	40
Euro OTC	Dicloridrato de histamina	2301007	26526	40
Euro OTC	Dicloridrato de histamina	2409007	27453	40
Fagron	Dicloridrato de histamina	15C25-B50-331242	23196	40
Fagron	Dicloridrato de histamina	22H25-B01-222394	26389	40
Euro OTC	Dicloridrato de histamina	2301007	26526SI	20
Euro OTC	Dicloridrato de histamina	2409007	27453SI	20
Fagron	Dicloridrato de histamina	15C25-B50-331242	23197	40
Fagron	Dicloridrato de histamina	22H25-B01-222394	26389SI	20

- 201 744 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 61 spectra from 32 *Apo-Ident* customers from 34 batches from the substance/substance group *Dicloridrato de histamina*.

- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Dicloridrato de histamina	1111004-02	1
Caelo	Dicloridrato de histamina	130500601	1
Euro OTC	Dicloridrato de histamina	1104004-03	1
Euro OTC	Dicloridrato de histamina	111004-02	1
Euro OTC	Dicloridrato de histamina	1111004-01	5
Euro OTC	Dicloridrato de histamina	1111004-02	1
Euro OTC	Dicloridrato de histamina	12K06-N08	2
Euro OTC	Dicloridrato de histamina	1305006-01	1
Euro OTC	Dicloridrato de histamina	1411012-02	4
Euro OTC	Dicloridrato de histamina	1411012-03	1
Euro OTC	Dicloridrato de histamina	1506030-01	3
Euro OTC	Dicloridrato de histamina	1811014-01	1
Euro OTC	Dicloridrato de histamina	1812018-01	1
Euro OTC	Dicloridrato de histamina	1905003-01	2
Euro OTC	Dicloridrato de histamina	1905003-02	3
Euro OTC	Dicloridrato de histamina	20021412	1
Euro OTC	Dicloridrato de histamina	2004012-01	1
Euro OTC	Dicloridrato de histamina	3031503	1
Fa Roth	Dicloridrato de histamina	47252901	1
Fagron	Dicloridrato de histamina	11E25-N07	2
Fagron	Dicloridrato de histamina	12D02-N16	1
Fagron	Dicloridrato de histamina	12E29-N09	3
Fagron	Dicloridrato de histamina	12K06-N08	5
Fagron	Dicloridrato de histamina	1305006-01	1
Fagron	Dicloridrato de histamina	14J06B01299179	1
Fagron	Dicloridrato de histamina	15E08-B06-313037	3
Fagron	Dicloridrato de histamina	17D11-B001-339451	1
Fagron	Dicloridrato de histamina	19D19-B02-361228	1
Fagron	Dicloridrato de histamina	28051305	1
Fagron	Dicloridrato de histamina	454545	1
Fagron	Dicloridrato de histamina	L17100130-OF-222030	1
Fargon/Fargon	Dicloridrato de histamina	19019-B02	1
Fargon/Fargon	Dicloridrato de histamina	19D19-B02	1
Fargon/Fargon	Dicloridrato de histamina	19H23-F04-364053	3
Merck	Dicloridrato de histamina	Wxbc3407V	1
Merck	Dicloridrato de histamina	WXBC3407V	1
Sanacop	Dicloridrato de histamina	15C25-B01-306047	1

- 236 006 spectra from 1515 *Apo-Ident* customers from a total of 49 225 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dicloridrato de histamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dicloridrato de histamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	340	0	201 744
Type C	0	61	0	236 006

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Dicloridrato de histamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2353 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.1639 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20963	20963	0,00	154,87
21668	21863	11,73	158,77
21863	21863	0,00	155,50
24589	25166	6,94	154,49
25166	25166	0,00	154,59
25413	25413	0,00	152,70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dicloridrato de octenidina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20759-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dicloridrato de octenidina; Octenidina, dicloridrato; Octenidini dihydrochloridum

Special notes

When selecting the *Dicloridrato de octenidina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dicloridrato de octenidina	10	4	246

Second-stage model

For differentiation of the substance/substance group *Dicloridrato de octenidina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dicloridrato de octenidina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	111,46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dicloridrato de octenidina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dicloridrato de octenidina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dicloridrato de octenidina	12115202	20759	40	20120511
Caelo	Dicloridrato de octenidina	13071407	20988	40	1407345
Caelo	Dicloridrato de octenidina	13166806	21331	40	20130718
Caelo	Dicloridrato de octenidina	15275502	21888	60	20150910
Caelo	Dicloridrato de octenidina	15356601	21947	60	1604116
Caelo	Dicloridrato de octenidina	15356601	21947SI	60	1604116
Caelo	Dicloridrato de octenidina	170423	23307	40	20170214*
Caelo	Dicloridrato de octenidina	170423	23307SI	40	20170214*
Caelo	Dicloridrato de octenidina	163355	23309	40	20170403*
Caelo	Dicloridrato de octenidina	18223413	24597	40	20181005
Caelo	Dicloridrato de octenidina	18223413	24597SI	40	20181005
Caelo	Dicloridrato de octenidina	23002809	27110	40	20240130*
Caelo	Dicloridrato de octenidina	24002081	27444	40	20240912*
Caelo	Dicloridrato de octenidina	24002081	27444SI	40	20240912*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 620 spectra of 14 reference samples from the substance/substance group *Dicloridrato de octenidina*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 342 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 10 reference samples from the substance/substance group *Dicloridrato de octenidina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dicloridrato de octenidina	160330	22485	60
Caelo	Dicloridrato de octenidina	180174	24023	40
Caelo	Dicloridrato de octenidina	20000606	25202	40
Caelo	Dicloridrato de octenidina	21002272	26010	40
Caelo	Dicloridrato de octenidina	15275502	21888SI†	60
Caelo	Dicloridrato de octenidina	163355	23309SI†	40
Caelo	Dicloridrato de octenidina	180174	24023SI	40
Caelo	Dicloridrato de octenidina	20000606	25202SI	40
Caelo	Dicloridrato de octenidina	21002272	26010SI	40
Caelo	Dicloridrato de octenidina	23002809	27110SI†	40

- 201 644 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2656 spectra from 881 *Apo-Ident* customers from 250 batches from the substance/substance group *Dicloridrato de octenidina*.
- Among them are spectra of independent samples from 246 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dicloridrato de octenidina	21002272002	1
	Dicloridrato de octenidina	21002272011	1
	Dicloridrato de octenidina	21002272012	6
	Dicloridrato de octenidina	21002272018	6
	Dicloridrato de octenidina	21002272020	1
	Dicloridrato de octenidina	21002272022	5
	Dicloridrato de octenidina	21002272024	5
	Dicloridrato de octenidina	21002272025	1
	Dicloridrato de octenidina	2102272024	1
	Dicloridrato de octenidina	22003039002	31
	Dicloridrato de octenidina	220030390021	1
	Dicloridrato de octenidina	22003039003	9
	Dicloridrato de octenidina	22003039004	9
	Dicloridrato de octenidina	22003039005	31
	Dicloridrato de octenidina	22003039008	2
	Dicloridrato de octenidina	22003039009	6
	Dicloridrato de octenidina	2203039002	2
	Dicloridrato de octenidina	23002809002	4
	Dicloridrato de octenidina	23002809003	2
	Dicloridrato de octenidina	23002809004	5
Aep	Dicloridrato de octenidina	22003039004	1
AHC	Dicloridrato de octenidina	20000606005	1
AHD	Dicloridrato de octenidina	16335507	1
AHD	Dicloridrato de octenidina	18197504	1
AHD	Dicloridrato de octenidina	20000606009	1
AHD	Dicloridrato de octenidina	21002272012	2
AHD	Dicloridrato de octenidina	21002272024	2
AHD	Dicloridrato de octenidina	22003039005	5
AHD	Dicloridrato de octenidina	23002809003	1
Alliance Healthcare	Dicloridrato de octenidina	18223403	3
Alliance Healthcare	Dicloridrato de octenidina	18223415	1
Alliance Healthcare	Dicloridrato de octenidina	21002272024	1
Alliance Healthcare	Dicloridrato de octenidina	22003039005	1
Alliance	Dicloridrato de octenidina	22003039002	2
Anzag	Dicloridrato de octenidina	17042602	1
Anzag	Dicloridrato de octenidina	20004187003	2
apomix	Dicloridrato de octenidina	13166813	1
Audor Pharma	Dicloridrato de octenidina	17042304	1
Bombastus	Dicloridrato de octenidina	17218506	1
Bombastus	Dicloridrato de octenidina	18017402	1
Cae	Dicloridrato de octenidina	21002272002	1
Caelo	Dicloridrato de octenidina		1
Caelo	Dicloridrato de octenidina	10(20000606019)	1
Caelo	Dicloridrato de octenidina	1000609006	1
Caelo	Dicloridrato de octenidina	11(20004187011)	1
Caelo	Dicloridrato de octenidina	11071925	1
Caelo	Dicloridrato de octenidina	12(20004187011)	1
Caelo	Dicloridrato de octenidina	13061801	1
Caelo	Dicloridrato de octenidina	13166801	1
Caelo	Dicloridrato de octenidina	13166808	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dicloridrato de octenidina	13166810	1
Caelo	Dicloridrato de octenidina	15006202	3
Caelo	Dicloridrato de octenidina	15006203	1
Caelo	Dicloridrato de octenidina	15006207	5
Caelo	Dicloridrato de octenidina	1515E-03732	1
Caelo	Dicloridrato de octenidina	15275502	8
Caelo	Dicloridrato de octenidina	152755020	1
Caelo	Dicloridrato de octenidina	15275503	3
Caelo	Dicloridrato de octenidina	15275504	1
Caelo	Dicloridrato de octenidina	15356601	6
Caelo	Dicloridrato de octenidina	15356603	4
Caelo	Dicloridrato de octenidina	15356702	1
Caelo	Dicloridrato de octenidina	15356703	9
Caelo	Dicloridrato de octenidina	16032803	8
Caelo	Dicloridrato de octenidina	16032901	2
Caelo	Dicloridrato de octenidina	16032902	4
Caelo	Dicloridrato de octenidina	16032903	2
Caelo	Dicloridrato de octenidina	16032909	7
Caelo	Dicloridrato de octenidina	16032910	6
Caelo	Dicloridrato de octenidina	16033001	2
Caelo	Dicloridrato de octenidina	16033002	2
Caelo	Dicloridrato de octenidina	16277802	9
Caelo	Dicloridrato de octenidina	16302910	1
Caelo	Dicloridrato de octenidina	16325202	1
Caelo	Dicloridrato de octenidina	16325304	11
Caelo	Dicloridrato de octenidina	16325305	14
Caelo	Dicloridrato de octenidina	16325406	6
Caelo	Dicloridrato de octenidina	16325408	2
Caelo	Dicloridrato de octenidina	16325410	3
Caelo	Dicloridrato de octenidina	16335502	3
Caelo	Dicloridrato de octenidina	16335504	23
Caelo	Dicloridrato de octenidina	16335505	4
Caelo	Dicloridrato de octenidina	16335506	1
Caelo	Dicloridrato de octenidina	16335507	11
Caelo	Dicloridrato de octenidina	16335508	8
Caelo	Dicloridrato de octenidina	16335509	20
Caelo	Dicloridrato de octenidina	16335510	12
Caelo	Dicloridrato de octenidina	17042302	8
Caelo	Dicloridrato de octenidina	17042303	6
Caelo	Dicloridrato de octenidina	17042304	13
Caelo	Dicloridrato de octenidina	17042305	5
Caelo	Dicloridrato de octenidina	17042501	1
Caelo	Dicloridrato de octenidina	17042601	1
Caelo	Dicloridrato de octenidina	17042602	9
Caelo	Dicloridrato de octenidina	17042701	1
Caelo	Dicloridrato de octenidina	17042903	21
Caelo	Dicloridrato de octenidina	1711160HC/16335509	1
Caelo	Dicloridrato de octenidina	172118501	1
Caelo	Dicloridrato de octenidina	17218051	1
Caelo	Dicloridrato de octenidina	17218501	45
Caelo	Dicloridrato de octenidina	17218503	15
Caelo	Dicloridrato de octenidina	172185035514	1
Caelo	Dicloridrato de octenidina	17218504	1
Caelo	Dicloridrato de octenidina	17218506	26
Caelo	Dicloridrato de octenidina	17218507	16
Caelo	Dicloridrato de octenidina	17218508	31
Caelo	Dicloridrato de octenidina	17218509	37
Caelo	Dicloridrato de octenidina	17218907	1
Caelo	Dicloridrato de octenidina	1728506	1
Caelo	Dicloridrato de octenidina	1728508	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dicloridrato de octenidina	18017402	74
Caelo	Dicloridrato de octenidina	18017404	1
Caelo	Dicloridrato de octenidina	18197501	52
Caelo	Dicloridrato de octenidina	18197502	23
Caelo	Dicloridrato de octenidina	181975025789	1
Caelo	Dicloridrato de octenidina	18197503	1
Caelo	Dicloridrato de octenidina	18197504	20
Caelo	Dicloridrato de octenidina	181987504	1
Caelo	Dicloridrato de octenidina	18223401	5
Caelo	Dicloridrato de octenidina	18223403	66
Caelo	Dicloridrato de octenidina	18223404	40
Caelo	Dicloridrato de octenidina	18223407	8
Caelo	Dicloridrato de octenidina	18223409	45
Caelo	Dicloridrato de octenidina	18223410	7
Caelo	Dicloridrato de octenidina	18223411	24
Caelo	Dicloridrato de octenidina	18223413	50
Caelo	Dicloridrato de octenidina	18223414	3
Caelo	Dicloridrato de octenidina	18223415	33
Caelo	Dicloridrato de octenidina	18223416	34
Caelo	Dicloridrato de octenidina	18223418	4
Caelo	Dicloridrato de octenidina	18223419	15
Caelo	Dicloridrato de octenidina	18223420	4
Caelo	Dicloridrato de octenidina	18223423	40
Caelo	Dicloridrato de octenidina	18223424	34
Caelo	Dicloridrato de octenidina	18223425	1
Caelo	Dicloridrato de octenidina	18223426	19
Caelo	Dicloridrato de octenidina	18223427	15
Caelo	Dicloridrato de octenidina	18223428	4
Caelo	Dicloridrato de octenidina	1822413	1
Caelo	Dicloridrato de octenidina	18233427	1
Caelo	Dicloridrato de octenidina	1823419	1
Caelo	Dicloridrato de octenidina	190118-03	1
Caelo	Dicloridrato de octenidina	2(18223413)	1
Caelo	Dicloridrato de octenidina	2000006016	1
Caelo	Dicloridrato de octenidina	200000606001	1
Caelo	Dicloridrato de octenidina	200000606005	2
Caelo	Dicloridrato de octenidina	200000606006	2
Caelo	Dicloridrato de octenidina	200000606011	1
Caelo	Dicloridrato de octenidina	200000606012	2
Caelo	Dicloridrato de octenidina	200000606016	2
Caelo	Dicloridrato de octenidina	200004187011	1
Caelo	Dicloridrato de octenidina	2000060002	1
Caelo	Dicloridrato de octenidina	2000060060011	1
Caelo	Dicloridrato de octenidina	200006012	1
Caelo	Dicloridrato de octenidina	20000605007	1
Caelo	Dicloridrato de octenidina	20000606001	31
Caelo	Dicloridrato de octenidina	20000606002	42
Caelo	Dicloridrato de octenidina	20000606005	25
Caelo	Dicloridrato de octenidina	20000606006	55
Caelo	Dicloridrato de octenidina	20000606007	11
Caelo	Dicloridrato de octenidina	20000606008	2
Caelo	Dicloridrato de octenidina	20000606009	17
Caelo	Dicloridrato de octenidina	2000060601	1
Caelo	Dicloridrato de octenidina	20000606010	1
Caelo	Dicloridrato de octenidina	20000606011	28
Caelo	Dicloridrato de octenidina	20000606012	29
Caelo	Dicloridrato de octenidina	20000606015	3
Caelo	Dicloridrato de octenidina	20000606016	23
Caelo	Dicloridrato de octenidina	20000606017	1
Caelo	Dicloridrato de octenidina	20000606018	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dicloridrato de octenidina	20000606019	44
Caelo	Dicloridrato de octenidina	2000060602	1
Caelo	Dicloridrato de octenidina	20000606022	3
Caelo	Dicloridrato de octenidina	2000060606	1
Caelo	Dicloridrato de octenidina	2000060611	1
Caelo	Dicloridrato de octenidina	2000060616	1
Caelo	Dicloridrato de octenidina	2000060619	1
Caelo	Dicloridrato de octenidina	20000620002	7
Caelo	Dicloridrato de octenidina	20004107016	1
Caelo	Dicloridrato de octenidina	2000418012	1
Caelo	Dicloridrato de octenidina	20004187001	29
Caelo	Dicloridrato de octenidina	20004187002	28
Caelo	Dicloridrato de octenidina	20004187003	29
Caelo	Dicloridrato de octenidina	20004187004	4
Caelo	Dicloridrato de octenidina	20004187006	6
Caelo	Dicloridrato de octenidina	20004187009	20
Caelo	Dicloridrato de octenidina	2000418701	1
Caelo	Dicloridrato de octenidina	20004187010	2
Caelo	Dicloridrato de octenidina	20004187011	27
Caelo	Dicloridrato de octenidina	20004187012	31
Caelo	Dicloridrato de octenidina	20004187013	7
Caelo	Dicloridrato de octenidina	20004187014	16
Caelo	Dicloridrato de octenidina	20004187015	23
Caelo	Dicloridrato de octenidina	20004187015(2x)	1
Caelo	Dicloridrato de octenidina	20004187016	15
Caelo	Dicloridrato de octenidina	20004187017	12
Caelo	Dicloridrato de octenidina	2000418704	1
Caelo	Dicloridrato de octenidina	200041871002	1
Caelo	Dicloridrato de octenidina	20004187101	1
Caelo	Dicloridrato de octenidina	200048187006	1
Caelo	Dicloridrato de octenidina	2000606001	1
Caelo	Dicloridrato de octenidina	2000606002	1
Caelo	Dicloridrato de octenidina	2000606006	1
Caelo	Dicloridrato de octenidina	2000606011	1
Caelo	Dicloridrato de octenidina	2000606012	1
Caelo	Dicloridrato de octenidina	2000606019	3
Caelo	Dicloridrato de octenidina	2000606021	1
Caelo	Dicloridrato de octenidina	200060612	1
Caelo	Dicloridrato de octenidina	2000620002	1
Caelo	Dicloridrato de octenidina	2004187002	1
Caelo	Dicloridrato de octenidina	2004187003	2
Caelo	Dicloridrato de octenidina	2004187006	1
Caelo	Dicloridrato de octenidina	2004187009	3
Caelo	Dicloridrato de octenidina	2004187011	1
Caelo	Dicloridrato de octenidina	2100227014	2
Caelo	Dicloridrato de octenidina	21002272001	4
Caelo	Dicloridrato de octenidina	21002272002	23
Caelo	Dicloridrato de octenidina	21002272003	16
Caelo	Dicloridrato de octenidina	21002272004	23
Caelo	Dicloridrato de octenidina	21002272006	12
Caelo	Dicloridrato de octenidina	21002272009	7
Caelo	Dicloridrato de octenidina	21002272011	1
Caelo	Dicloridrato de octenidina	21002272012	7
Caelo	Dicloridrato de octenidina	21002272014	16
Caelo	Dicloridrato de octenidina	21002272015	5
Caelo	Dicloridrato de octenidina	21002272018	13
Caelo	Dicloridrato de octenidina	2100227202	1
Caelo	Dicloridrato de octenidina	21002272020	1
Caelo	Dicloridrato de octenidina	21002272022	11
Caelo	Dicloridrato de octenidina	21002272024	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dicloridrato de octenidina	21002272025	1
Caelo	Dicloridrato de octenidina	2100272020	1
Caelo	Dicloridrato de octenidina	210906(20004187011)	1
Caelo	Dicloridrato de octenidina	211002272004	1
Caelo	Dicloridrato de octenidina	22003039002	7
Caelo	Dicloridrato de octenidina	22003039005	1
Caelo	Dicloridrato de octenidina	220516(21002272002)	1
Caelo	Dicloridrato de octenidina	220622(21002272002)	1
Caelo	Dicloridrato de octenidina	221222/5	1
Caelo	Dicloridrato de octenidina	2304187009	1
Caelo	Dicloridrato de octenidina	2x2004187002	1
Caelo	Dicloridrato de octenidina	300718A	1
Caelo	Dicloridrato de octenidina	3277	1
Caelo	Dicloridrato de octenidina	3329	1
Caelo	Dicloridrato de octenidina	606007	1
Caelo	Dicloridrato de octenidina	606019	1
Caelo	Dicloridrato de octenidina	6325305	1
Caelo	Dicloridrato de octenidina	718A-03273	1
Caelo	Dicloridrato de octenidina	816M-03732	1
Caelo	Dicloridrato de octenidina	8724	1
Caesar & Lorenz GmbH	Dicloridrato de octenidina	16325410	1
Caesar & Lorenz GmbH	Dicloridrato de octenidina	17218503	1
Caesar & Lorenz GmbH	Dicloridrato de octenidina	18223416	2
Caesar & Lorenz GmbH	Dicloridrato de octenidina	200006006	1
Caesar & Lorenz GmbH	Dicloridrato de octenidina	20000606001	1
Caesar & Lorenz GmbH	Dicloridrato de octenidina	20000606005	1
Caesar & Loretz / Sa...	Dicloridrato de octenidina	18223404	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	16325305	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223403	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187009	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272004	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187002	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272014	2
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223403	2
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223415	2
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223428	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18233415	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606005	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606006	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606012	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223416	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223426	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606002	1
Caesar & Loretz GmbH/ G	Dicloridrato de octenidina	18223404	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187014	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606002	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187018	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187002	1
Caesar & Loretz GmbH/	Dicloridrato de octenidina	21002272002	1
Caesar & Loretz GmbH/AEP	Dicloridrato de octenidina	20000606009	1
Caesar & Loretz GmbH/AEP	Dicloridrato de octenidina	20004187015	1
Caesar & Loretz GmbH/AHD	Dicloridrato de octenidina	20000606012	1
Caesar & Loretz GmbH/AHD	Dicloridrato de octenidina	21002272003	1
Caesar & Loretz GmbH/AHD	Dicloridrato de octenidina	21002272018	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606011	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223423	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606011	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606012	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187011	1
Caesar & Loretz GmbH/G	Dicloridrato de octenidina	20004187003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	18223413	1
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	20000606006	1
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	20000606009	1
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	20000606010	1
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	20000606012	1
Caesar & Loretz GmbH/GEHE	Dicloridrato de octenidina	20000606012	1
Caesar & Loretz GmbH/GEHE	Dicloridrato de octenidina	20000606018	1
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	20004187003	4
Caesar & Loretz GmbH/Gehe	Dicloridrato de octenidina	20004187009	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187012	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187002	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223411	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606002	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606005	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606016	2
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187001	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272011	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272014	2
Caesar & Loretz GmbH/K	Dicloridrato de octenidina	20004187013	1
Caesar & Loretz GmbH/Kehr	Dicloridrato de octenidina	18223418	1
Caesar & Loretz GmbH/Kehr	Dicloridrato de octenidina	21002272025	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223425	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187015	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223423	2
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606006	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606015	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606019	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187002	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187015	3
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187016	3
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272022	2
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272003	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272004	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223416	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223423	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20000606019	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187003	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187006	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	21002272003	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	22003039002	1
Caesar & Loretz GmbH/S	Dicloridrato de octenidina	20004187016	1
Caesar & Loretz GmbH/Sana	Dicloridrato de octenidina	18223415	1
Caesar & Loretz GmbH/Sana	Dicloridrato de octenidina	20000606006	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223411	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	18223427	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187001	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187003	1
Caesar & Loretz GmbH...	Dicloridrato de octenidina	20004187016	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	15006210	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	17218509	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	18017404	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	181975002	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	18197502	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223403	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223404	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223409	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223411	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223413	7
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223415	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223416	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223419	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223420	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223423	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223424	7
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223426	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223427	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	18223428	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	200006001	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606001	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606002	9
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606005	9
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606006	12
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606007	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606009	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606010	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606011	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606012	7
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606015	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606016	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606019	18
Caesar & Loretz GmbH	Dicloridrato de octenidina	20000606022	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	200006066005	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187001	9
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187002	18
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187003	13
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187006	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187009	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187010	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187011	10
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187012	8
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187013	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187014	7
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187015	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187016	7
Caesar & Loretz GmbH	Dicloridrato de octenidina	20004187017	8
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272002	9
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272003	8
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272004	9
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272006	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272009	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272011	3
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272012	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272014	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272018	5
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272020	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272022	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272024	4
Caesar & Loretz GmbH	Dicloridrato de octenidina	21002272025	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	22003039002	1
Caesar & Loretz GmbH	Dicloridrato de octenidina	22003039004	2
Caesar & Loretz GmbH	Dicloridrato de octenidina	22003039005	2
Caesar & Loretz Hild...	Dicloridrato de octenidina	20000606005	2
Caesar & Loretz Hild...	Dicloridrato de octenidina	18223403	2
Caesar & Loretz Hild...	Dicloridrato de octenidina	18223413	1
Caesar & Loretz Hild...	Dicloridrato de octenidina	183223424	1
Caesar & Loretz Hild...	Dicloridrato de octenidina	20000606012	1
Caesar & Loretz Hild...	Dicloridrato de octenidina	20000606019	1
Caesar & Loretz Hilden	Dicloridrato de octenidina	18223416	1
Caesar & Loretz Hilden	Dicloridrato de octenidina	20000606006	2
Caesar & Loretz/AHD	Dicloridrato de octenidina	20000606001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz/Noweda	Dicloridrato de octenidina	20000606019	1
Caesar & Loretz/Noweda	Dicloridrato de octenidina	20004187002	1
Caesar & Loretz	Dicloridrato de octenidina	232215	1
Caesar&Lorenz / Gehe	Dicloridrato de octenidina	18223419	1
Caesar&Lorenz/AHD	Dicloridrato de octenidina	17218508	1
Caesar&Lorenz	Dicloridrato de octenidina	2000487017	1
Caesar&Loretz GmbH, ...	Dicloridrato de octenidina	17042302	1
Caesar&Loretz GmbH	Dicloridrato de octenidina	16335504	1
Caesar&Loretz GmbH	Dicloridrato de octenidina	20000606011	1
Caesar&Loretz GmbH	Dicloridrato de octenidina	21002272011	1
Caleo/ Fiebig	Dicloridrato de octenidina	17218508	2
CALEO/Noweda	Dicloridrato de octenidina	20000606006	1
Caleo	Dicloridrato de octenidina	16033001	1
Caleo	Dicloridrato de octenidina	18197504	1
Caleo	Dicloridrato de octenidina	18223409	1
Caleo	Dicloridrato de octenidina	2000606001	1
Calo, Hilden/ Phönix	Dicloridrato de octenidina	20004187012	1
Calo/Gehe	Dicloridrato de octenidina	16335508	1
Calo/Gehe	Dicloridrato de octenidina	18223404	1
carelo	Dicloridrato de octenidina	22003039005	1
Cealo/Anzag	Dicloridrato de octenidina	211203(20004187015)	1
Cealo/Sanacorp	Dicloridrato de octenidina	15006207	1
Cealo/Sanacorp	Dicloridrato de octenidina	16325305	1
Cealo	Dicloridrato de octenidina	17218507	1
Cealo	Dicloridrato de octenidina	20000606001	1
Cealo5440	Dicloridrato de octenidina	17218501	1
Ceasar & Loretz GmbH...	Dicloridrato de octenidina	16335509	1
Ceasar & Loretz	Dicloridrato de octenidina	20004187012	3
Celo	Dicloridrato de octenidina	16277802	1
Celo	Dicloridrato de octenidina	20000606006	2
Ebert & Jacobi	Dicloridrato de octenidina	16032902	1
Ebert & Jacobi	Dicloridrato de octenidina	16325406	1
EuRho/ AHD	Dicloridrato de octenidina	17218507	1
EuRho/Sanacorp	Dicloridrato de octenidina	16335508	1
Euro OTC	Dicloridrato de octenidina	16032803	1
Euro OTC	Dicloridrato de octenidina	17218501	1
Euro OTC	Dicloridrato de octenidina	18197502	2
Euro OTC	Dicloridrato de octenidina	18223404	1
Euro OTC	Dicloridrato de octenidina	18223413	4
Euro OTC	Dicloridrato de octenidina	20004187014	1
Fagron	Dicloridrato de octenidina	15356601	1
Fagron	Dicloridrato de octenidina	15356703	1
Fagron	Dicloridrato de octenidina	16277802	1
Fagron	Dicloridrato de octenidina	16335507	1
Fagron	Dicloridrato de octenidina	16335510	1
Fagron	Dicloridrato de octenidina	18017402	1
Fagron	Dicloridrato de octenidina	18197501	3
Fagron	Dicloridrato de octenidina	18223403	2
Fagron	Dicloridrato de octenidina	187223403	1
Fagron	Dicloridrato de octenidina	18A12-B03-346964	1
Ferak / Caesar & Lor...	Dicloridrato de octenidina	18197502	1
Ferak Berlin GmbH/ AHD	Dicloridrato de octenidina	20000620002	1
Ferak/Noweda	Dicloridrato de octenidina	202120	1
Ferak/Phoenix	Dicloridrato de octenidina	62120	1
Fiebig	Dicloridrato de octenidina	18017402	1
Fiebig	Dicloridrato de octenidina	20000606009	1
Fresenius	Dicloridrato de octenidina	60715101	1
Gehe 21-01-2019	Dicloridrato de octenidina	18223403	1
Gehe amax	Dicloridrato de octenidina	15356603	1
Gehe amax	Dicloridrato de octenidina	15356703	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe amax	Dicloridrato de octenidina	16325305	1
Gehe amax	Dicloridrato de octenidina	17042305	1
Gehe amax	Dicloridrato de octenidina	17218509	1
Gehe amax	Dicloridrato de octenidina	18197501	1
Gehe amax	Dicloridrato de octenidina	20000606006	1
Gehe Rostock	Dicloridrato de octenidina	18223427	1
Gehe Rostock	Dicloridrato de octenidina	21002272022	1
Gehe	Dicloridrato de octenidina	16032909	2
GEHE	Dicloridrato de octenidina	16325304	1
GEHE	Dicloridrato de octenidina	16325305	1
Gehe	Dicloridrato de octenidina	16335502	1
gehe	Dicloridrato de octenidina	17042602	1
Gehe	Dicloridrato de octenidina	17042903	1
Gehe	Dicloridrato de octenidina	17218501	1
Gehe	Dicloridrato de octenidina	17218508	1
GEHE	Dicloridrato de octenidina	17218509	1
Gehe	Dicloridrato de octenidina	172218508	1
Gehe	Dicloridrato de octenidina	18017402	2
Gehe	Dicloridrato de octenidina	18223401	1
Gehe	Dicloridrato de octenidina	18223403	1
Gehe	Dicloridrato de octenidina	18223419	1
Gehe	Dicloridrato de octenidina	18223424	1
Gehe	Dicloridrato de octenidina	20000606018	1
Gehe	Dicloridrato de octenidina	20004187003	1
gehe	Dicloridrato de octenidina	20004187016	1
Gehe	Dicloridrato de octenidina	20004187016	1
Gehe	Dicloridrato de octenidina	21002272018	1
Gehe	Dicloridrato de octenidina	21002272022	1
Gehe	Dicloridrato de octenidina	21002272024	1
Gehe	Dicloridrato de octenidina	22003039002	2
Gehe	Dicloridrato de octenidina	22003039004	1
Gehe	Dicloridrato de octenidina	22003039005	3
Hepart	Dicloridrato de octenidina	17218508	1
Jenne	Dicloridrato de octenidina	17218507	1
JENNE	Dicloridrato de octenidina	17218508	1
Jenne	Dicloridrato de octenidina	18197502	2
Jenne	Dicloridrato de octenidina	18223416	1
Jenne	Dicloridrato de octenidina	20004187009	1
Kehr	Dicloridrato de octenidina	17218508	1
Kehr	Dicloridrato de octenidina	21002272014	1
Kehr	Dicloridrato de octenidina	21002272018	2
Kehr	Dicloridrato de octenidina	22003039002	2
Kehr	Dicloridrato de octenidina	22003039003	1
Kehr	Dicloridrato de octenidina	22003039004	1
Kehr	Dicloridrato de octenidina	22003039005	1
Kehr	Dicloridrato de octenidina	22003039009	1
Krieger	Dicloridrato de octenidina	20000606019	1
Krieger	Dicloridrato de octenidina	3132	1
Löwen City-Apotheke ...	Dicloridrato de octenidina	2042015	1
Noweda /Cealo	Dicloridrato de octenidina	20000606006	1
Noweda	Dicloridrato de octenidina	16335507	1
Noweda	Dicloridrato de octenidina	17218501	1
Noweda	Dicloridrato de octenidina	18223403	1
Noweda	Dicloridrato de octenidina	18223415	1
Noweda	Dicloridrato de octenidina	18223420	2
Noweda	Dicloridrato de octenidina	1822419	1
Noweda	Dicloridrato de octenidina	20000606019	1
Noweda	Dicloridrato de octenidina	20004187001	1
Noweda	Dicloridrato de octenidina	20004187016	2
Noweda	Dicloridrato de octenidina	20004187017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Dicloridrato de octenidina	2004187009	1
Noweda	Dicloridrato de octenidina	21002272003no	1
Noweda	Dicloridrato de octenidina	21002272012	1
Noweda	Dicloridrato de octenidina	21002272014	1
Noweda	Dicloridrato de octenidina	21002272024	2
Noweda	Dicloridrato de octenidina	220030309005	1
Noweda	Dicloridrato de octenidina	22003039002	1
Noweda	Dicloridrato de octenidina	22003039005	2
noweda	Dicloridrato de octenidina	22003039008	1
Pheonix	Dicloridrato de octenidina	17218509	1
Phoenix	Dicloridrato de octenidina	17218506	1
Phoenix	Dicloridrato de octenidina	18223415	2
Phoenix	Dicloridrato de octenidina	20000606016	1
Phoenix	Dicloridrato de octenidina	20004187003	2
Phoenix	Dicloridrato de octenidina	20004187016	1
Phoenix	Dicloridrato de octenidina	22003039002	1
Phoenix	Dicloridrato de octenidina	22003039004	1
Phoenix	Dicloridrato de octenidina	22003039005	3
Phoenix	Dicloridrato de octenidina	3033	1
Phoenix	Dicloridrato de octenidina	3040	1
Phoenix	Dicloridrato de octenidina	3107	1
Phoenix	Dicloridrato de octenidina	3113	1
Phoenix	Dicloridrato de octenidina	3221	1
Phoenix	Dicloridrato de octenidina	3419	1
Phoenix	Dicloridrato de octenidina	3423	1
Phönix Gotha	Dicloridrato de octenidina	17218508	1
Phönix	Dicloridrato de octenidina	17218506	1
Phönix	Dicloridrato de octenidina	20000606011	1
Phönix	Dicloridrato de octenidina	20004187006	1
Phönix	Dicloridrato de octenidina	20004187013	1
Phönix	Dicloridrato de octenidina	2000606019	1
PHÖNIX	Dicloridrato de octenidina	21002272002	1
Phönix	Dicloridrato de octenidina	21002272006	1
Phönix	Dicloridrato de octenidina	21002272018	1
phönix	Dicloridrato de octenidina	22003039005	1
Phönix	Dicloridrato de octenidina	22003039005	7
Phönix	Dicloridrato de octenidina	23002809002	1
Phönix	Dicloridrato de octenidina	23002809004	1
Phönix	Dicloridrato de octenidina	3155	1
sanacorb	Dicloridrato de octenidina	18197502	1
Sanacorp	Dicloridrato de octenidina	16335504	1
Sanacorp	Dicloridrato de octenidina	17218509	1
Sanacorp	Dicloridrato de octenidina	18223426	1
Sanacorp	Dicloridrato de octenidina	22003039002	3
Sanacorp	Dicloridrato de octenidina	22003039005	1
Spangro	Dicloridrato de octenidina	17042305	1

- 233 411 spectra from 1515 *Apo-Ident* customers from a total of 49 012 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dicloridrato de octenidina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dicloridrato de octenidina*

and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	440	0	201 644
Type C	0	2582	74	233 411

The substance/substance group *Dicloridrato de octenidina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	97.2139 % (> 97.1009 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20759	27110	8,83	168,21
20988	20988	0,00	164,90
21331	21947	19,73	176,67
21888	21947	3,44	166,01
21947	21947	0,00	168,85
23307	23307	0,00	177,71
23309	23309	0,00	168,59
24597	27110	8,70	168,45
27110	27110	0,00	168,52
27444	27444	0,00	174,87

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Difenilciclopropenona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10003690-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Difenilciclopropenona; Difenciprona; Diphenylcyclopropenonum

Special notes

When selecting the *Difenilciclopropenona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Difenilciclopropenona	7	3	12

Second-stage model

For differentiation of the substance/substance group *Difenilciclopropenona* the following second-stage model is used:

- Submodelo 18

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Difenilciclopropenona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Benzoato de sódio	45,05	27,24
Ditranol	113,76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Difenilciclopropenona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Difenilciclopropenona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Difenilciclopropenona	12L17-N07	20934	40	1407599
Fagron	Difenilciclopropenona	13I26-N12	21342	40	1504598
Fagron	Difenilciclopropenona	13I26-N12	21539	35	20130920
Fagron	Difenilciclopropenona	16F02-B10-329708	23070	40	1902476
Fagron	Difenilciclopropenona	16F02-B10-326265	23071	40	20160822
Fagron	Difenilciclopropenona	20I09-F02-374243	25585	40	20201016
Fagron	Difenilciclopropenona	20J27-F06-374823	25741	50	20201109
Fagron	Difenilciclopropenona	22D27-B01-226151	26540	40	20220630
Fagron	Difenilciclopropenona	22D27-B01-226151	26540SI	20	20220630

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 345 spectra of 9 reference samples from the substance/substance group *Difenilciclopropenona*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 617 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 3 reference samples from the substance/substance group *Difenilciclopropenona*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Difenilciclopropenona	15J12-B01-316620	22362	60
Fagron	Difenilciclopropenona	18I03-B04-356833	24582	40
Fagron	Difenilciclopropenona	19K26-F01-367396	25189	40

- 201 944 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 13 *Apo-Ident* customers from 13 batches from the substance/substance group *Difenilciclopropenona*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Difenilciclopropenona	17B-13B02-334769	1
Fagron	Difenilciclopropenona	1(17B13-B02-34977)	1
Fagron	Difenilciclopropenona	16F02B10324263	1
Fagron	Difenilciclopropenona	16F02-B10-327812	3
Fagron	Difenilciclopropenona	18I03B04	1
Fagron	Difenilciclopropenona	18I-03-B04	1
Fagron	Difenilciclopropenona	18I03-B04_356833	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Difenilciclopropenona	19K26-F01-367396	1
Fagron	Difenilciclopropenona	20J27-F06-374823	1
Fagron	Difenilciclopropenona	35-16-I-95P3117	1
Fagron	Difenilciclopropenona	35-17-II-57P3503	1
Fiebig	Difenilciclopropenona	17B13-B02-334769	1
Frago/Noweda	Difenilciclopropenona	16F02-B10-324263	2

- 236 051 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Difenilciclopropenona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Difenilciclopropenona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	345	0	152 617
Type B	0	140	0	201 944
Type C	0	16	0	236 051

The substance/substance group *Difenilciclopropenona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2609 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20934	20934	0,00	102,33
21342	21342	0,00	274,97
21539	21342	4,51	283,16
23070	23070	0,00	93,22
23071	21342	64,38	277,20
25585	20934	35,56	113,62
25741	20934	12,55	107,77
26540	20934	39,01	96,11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Di-hidrocodeína[(R,R)-tartarato]**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20303-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Di-hidrocodeína[(R,R)-tartarato]; Di-hidrocodeína, tartarato; Dihydrocodeini hydrogenotartras

Special notes

When selecting the *Di-hidrocodeína[(R,R)-tartarato]* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Di-hidrocodeína[(R,R)-tartarato]	8	3	42

Second-stage model

For differentiation of the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	56,05	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Di-hidrocodeína[(R,R)-tar…	13267601	21156	40	0914A-03065
Caelo	Di-hidrocodeína[(R,R)-tar…	13267601	21156SI	60	0914A-03065
Caelo	Di-hidrocodeína[(R,R)-tar…	12142506	21158	40	0914B-03065
Caelo	Di-hidrocodeína[(R,R)-tar…	12142506	21158SI	60	0914B-03065
Caelo	Di-hidrocodeína[(R,R)-tar…	15295901	22418	60	1316Q-03065
Caelo	Di-hidrocodeína[(R,R)-tar…	15295901	22418SI	60	1316Q-03065
Fagron	Di-hidrocodeína[(R,R)-tar…	13H19-N03	21160	40	0914C-03065
Fagron	Di-hidrocodeína[(R,R)-tar…	13H19-N03	21160SI	60	0914C-03065
Fagron	Di-hidrocodeína[(R,R)-tar…	14K26-B04-306298	22422	60	1516I-03065
Fagron	Di-hidrocodeína[(R,R)-tar…	15F18-B07-323388	23479	40	2017A-03065
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	67035	21162	40	0914D-03065
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	67035	21162SI	60	0914D-03065
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	067052	23476	40	2017D-03065

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 660 spectra of 13 reference samples from the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 302 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 9 reference samples from the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Di-hidrocodeína[(R,R)-tar…	16106209	23477	40
Caelo	Di-hidrocodeína[(R,R)-tar…	15295910	23478	40
Caelo	Di-hidrocodeína[(R,R)-tar…	18115205	24651	40
Caelo	Di-hidrocodeína[(R,R)-tar…	16106209	23477SI	40
Caelo	Di-hidrocodeína[(R,R)-tar…	15295910	23478SI	40
Caelo	Di-hidrocodeína[(R,R)-tar…	18115205	24651SI	40
Fagron	Di-hidrocodeína[(R,R)-tar…	14K26-B04-306298	22422SI†	60
Fagron	Di-hidrocodeína[(R,R)-tar…	15F18-B07-323388	23479SI†	40
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	067052	23476SI†	40

- 201 704 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 91 spectra from 16 *Apo-Ident* customers from 45 batches from the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 42 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Di-hidrocodeína[(R,R)-tar…	21F03-F02-379260	3
	Di-hidrocodeína[(R,R)-tar…	3020321	2
Caelo	Di-hidrocodeína[(R,R)-tar…	12142503	2
Caelo	Di-hidrocodeína[(R,R)-tar…	12142508	2
Caelo	Di-hidrocodeína[(R,R)-tar…	13267603	1
Caelo	Di-hidrocodeína[(R,R)-tar…	13267604	2
Caelo	Di-hidrocodeína[(R,R)-tar…	13267608	1
Caelo	Di-hidrocodeína[(R,R)-tar…	15295903	2
Caelo	Di-hidrocodeína[(R,R)-tar…	15295905	4
Caelo	Di-hidrocodeína[(R,R)-tar…	15295907	1
Caelo	Di-hidrocodeína[(R,R)-tar…	15F18-B07-322054	1
Caelo	Di-hidrocodeína[(R,R)-tar…	16106202	5
Caelo	Di-hidrocodeína[(R,R)-tar…	16106203	4
Caelo	Di-hidrocodeína[(R,R)-tar…	17097502	2
Caelo	Di-hidrocodeína[(R,R)-tar…	17097508	2
Caelo	Di-hidrocodeína[(R,R)-tar…	18115202	3
Caelo	Di-hidrocodeína[(R,R)-tar…	18115205	2
Caelo	Di-hidrocodeína[(R,R)-tar…	19D15-B02-363307	1
Caesar & Loretz GmbH	Di-hidrocodeína[(R,R)-tar…	192004005	1
Caesar & Loretz GmbH	Di-hidrocodeína[(R,R)-tar…	20003430003	1
Caesar & Loretz GmbH	Di-hidrocodeína[(R,R)-tar…	20003430006	1
Fagron	Di-hidrocodeína[(R,R)-tar…	12G05-N01	1
Fagron	Di-hidrocodeína[(R,R)-tar…	13H19-N08	3
Fagron	Di-hidrocodeína[(R,R)-tar…	14D08-B06	1
Fagron	Di-hidrocodeína[(R,R)-tar…	14K26-B04	1
Fagron	Di-hidrocodeína[(R,R)-tar…	14K26-B04-310974	1
Fagron	Di-hidrocodeína[(R,R)-tar…	14K26-B04-317257	1
Fagron	Di-hidrocodeína[(R,R)-tar…	15F18B07	2
Fagron	Di-hidrocodeína[(R,R)-tar…	15F18-B07	1
Fagron	Di-hidrocodeína[(R,R)-tar…	15F18-B07-323388	1
Fagron	Di-hidrocodeína[(R,R)-tar…	16-00326	1
Fagron	Di-hidrocodeína[(R,R)-tar…	16I27-B03	1
Fagron	Di-hidrocodeína[(R,R)-tar…	16I27-B03-332122	1
Fagron	Di-hidrocodeína[(R,R)-tar…	17G04-B02	1
Fagron	Di-hidrocodeína[(R,R)-tar…	17G04-B02-342861	1
Fagron	Di-hidrocodeína[(R,R)-tar…	21f03-f02-379260	1
Fagron	Di-hidrocodeína[(R,R)-tar…	3080620	1
Fagron	Di-hidrocodeína[(R,R)-tar…	B02-3683109	1
Fagron	Di-hidrocodeína[(R,R)-tar…	F02-3756503	4
Hedinger	Di-hidrocodeína[(R,R)-tar…	70162	4
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	20170808-03065	1
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	59819	1
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	67035	2
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	67052	10
Th. Geyer	Di-hidrocodeína[(R,R)-tar…	70729	6

- 235 976 spectra from 1515 *Apo-Ident* customers from a total of 49 213 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Di-hidrocodeína[(R,R)-tartarato]* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Di-hidrocodeína[(R,R)-tartarato]* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	660	0	152 302
Type B	0	379	1	201 704
Type C	0	91	0	235 976

The substance/substance group *Di-hidrocodeína[(R,R)-tartarato]* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0909 %)
Type B	100.0000 % (> 99.9912 %)	99.7368 % (> 98.9474 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.4066 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21156	21156	0,00	147,19
21158	21158	0,00	146,02
21160	21160	0,00	146,41
21162	21162	0,00	139,13
22418	22418	0,00	144,64
22422	22422	0,00	145,08
23476	23476	0,00	137,17
23479	23479	0,00	141,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dihidrogenofosfato de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006389-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dihidrogenofosfato de potássio; Fosfato de potássio dibásico; Kalii dihydrogenophosphas

Special notes

When selecting the *Dihidrogenofosfato de potássio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dihidrogenofosfato de potássio	3	1	0

Second-stage model

For differentiation of the substance/substance group *Dihidrogenofosfato de potássio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dihidrogenofosfato de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Proteinato de prata	42,67	–
Carbômero	57,94	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dihidrogenofosfato de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dihidrogenofosfato de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dihidrogenofosfato de potássio	22001752	26567	40	20220615*
Caelo	Dihidrogenofosfato de potássio	22001752	26567SI	20	20220615*
Caelo	Dihidrogenofosfato de potássio	23003147	27113	40	20240118*
Caelo	Dihidrogenofosfato de potássio	23003147	27113SI	20	20240118*
Caelo	Dihidrogenofosfato de potássio	24002258	27446	40	20241014*
Caelo	Dihidrogenofosfato de potássio	24002258	27446SI	20	20241014*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 180 spectra of 6 reference samples from the substance/substance group *Dihidrogenofosfato de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 152 782 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Dihidrogenofosfato de potássio*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dihidrogenofosfato de potássio	172493	23689	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Dihidrogenofosfato de potássio*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dihidrogenofosfato de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For

this purpose, all relevant spectra of the various substances were compared with *Dihidrogenofosfato de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Dihidrogenofosfato de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26567	26567	0,00	59,48
27113	27113	0,00	56,77
27446	27446	0,00	57,54

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dinitrato de isossorbida 40%**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20213-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dinitrato de isossorbida 40%; Isorbidi dinitras 40%; Isossorbida, dinitrato 40%

Special notes

When selecting the *Dinitrato de isossorbida 40%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dinitrato de isossorbida 40%	5	3	229

Second-stage model

For differentiation of the substance/substance group *Dinitrato de isossorbida 40%* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dinitrato de isossorbida 40%* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	65,40	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dinitrato de isossorbida 40%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dinitrato de isossorbida 40%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Dinitrato de isossorbida 40%	12F08-N04	20891	40	20120801
Fagron	Dinitrato de isossorbida 40%	13D15-N02	21347	39	20130410
Fagron	Dinitrato de isossorbida 40%	15I10-B01-328577	23200	40	1709092
Fagron	Dinitrato de isossorbida 40%	15I10-B01-328577	23598	30	20150922
Fagron	Dinitrato de isossorbida 40%	17C29-B01-339447	24057	40	20170517
Fagron	Dinitrato de isossorbida 40%	23F19-B04-231383	27044	40	20231004

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 229 spectra of 6 reference samples from the substance/substance group *Dinitrato de isossorbida 40%*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 733 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Dinitrato de isossorbida 40%*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Dinitrato de isossorbida 40%	15I10-B01-315217	22762	40
Fagron	Dinitrato de isossorbida 40%	18J18-B01-363845	25065	40
Fagron	Dinitrato de isossorbida 40%	22D11-B05-215487	26300	40
Fagron	Dinitrato de isossorbida 40%	22D11-B05-215487	26300SI	10
Fagron	Dinitrato de isossorbida 40%	23F19-B04-231383	27044SI†	20

- 201 934 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1054 spectra from 437 *Apo-Ident* customers from 269 batches from the substance/substance group *Dinitrato de isossorbida 40%*.
- Among them are spectra of independent samples from 227 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dinitrato de isossorbida 40%		1
	Dinitrato de isossorbida 40%	17c29-b01-348859	1
	Dinitrato de isossorbida 40%	2203089	4
	Dinitrato de isossorbida 40%	22D11-B05-215487	1
	Dinitrato de isossorbida 40%	22D11-B05-216314	7

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Dinitrato de isossorbida 40%	22D11-B05-225756	2
	Dinitrato de isossorbida 40%	22D11-b05225757	1
	Dinitrato de isossorbida 40%	22D11-B05-225757	1
	Dinitrato de isossorbida 40%	22D11B05229443	1
	Dinitrato de isossorbida 40%	22D11-B05-229443	2
	Dinitrato de isossorbida 40%	23F19-B04-231383	1
	Dinitrato de isossorbida 40%	B0521631004	1
AEP GmbH	Dinitrato de isossorbida 40%	B01-3638405	1
AHD 09.03.2015	Dinitrato de isossorbida 40%	14D09-B03-294281	1
AHD	Dinitrato de isossorbida 40%	17C29-B01-350470	1
Ahd	Dinitrato de isossorbida 40%	2203089	1
AHD	Dinitrato de isossorbida 40%	22D11-B05-225757	5
AHD	Dinitrato de isossorbida 40%	23F19-B04-231383	1
Alliance / Fargon	Dinitrato de isossorbida 40%	18J18-B01-359177	2
Allianz Healthcare 1...	Dinitrato de isossorbida 40%	14D09-B03-300234	1
Anzag	Dinitrato de isossorbida 40%	12C08-N05	2
Anzag	Dinitrato de isossorbida 40%	15/10-B01-328577	1
Anzag	Dinitrato de isossorbida 40%	1510B01315217	1
apo-ident	Dinitrato de isossorbida 40%	18J18-B01-359177	1
Avara Shannon / Eber...	Dinitrato de isossorbida 40%	193469	2
Avara Shannon Pharm ...	Dinitrato de isossorbida 40%	195293	1
Avara Shannon Pharm....	Dinitrato de isossorbida 40%	18J18-B01-358247	1
Avara Shannon Pharm/ gehe	Dinitrato de isossorbida 40%	195293	1
Avara Shannon	Dinitrato de isossorbida 40%		1
Caelo	Dinitrato de isossorbida 40%		1
Caelo	Dinitrato de isossorbida 40%	11/17-N05	1
Caelo	Dinitrato de isossorbida 40%	11D12-N01	1
Caelo	Dinitrato de isossorbida 40%	13/26-N18	1
Caelo	Dinitrato de isossorbida 40%	13D15-N02	3
Caelo	Dinitrato de isossorbida 40%	13F27-N04	1
Caelo	Dinitrato de isossorbida 40%	149168	2
Caelo	Dinitrato de isossorbida 40%	14D09B03294281	1
Caelo	Dinitrato de isossorbida 40%	14D09-B03-294281	2
Caelo	Dinitrato de isossorbida 40%	14D-09-B03-300234	1
Caelo	Dinitrato de isossorbida 40%	14D09-B03-307018	1
Caelo	Dinitrato de isossorbida 40%	14D09-B03-308419	4
Caelo	Dinitrato de isossorbida 40%	15/10-B01-320081	4
Caelo	Dinitrato de isossorbida 40%	15/10-B01-325474	2
Caelo	Dinitrato de isossorbida 40%	15/10-B01-328577	1
Caelo	Dinitrato de isossorbida 40%	15/10-B01-331286	1
Caelo	Dinitrato de isossorbida 40%	1510-B01-315217	1
Caelo	Dinitrato de isossorbida 40%	1510-B01-320081	2
Caelo	Dinitrato de isossorbida 40%	15-10b01-328132	1
Caelo	Dinitrato de isossorbida 40%	15-10-b01-328132	2
Caelo	Dinitrato de isossorbida 40%	1510b1320782	1
Caelo	Dinitrato de isossorbida 40%	15I10-B01	1
Caelo	Dinitrato de isossorbida 40%	15I10-B01-328577	1
Caelo	Dinitrato de isossorbida 40%	15l10-B01-325474	1
Caelo	Dinitrato de isossorbida 40%	17C29-B01-335070	2
Caelo	Dinitrato de isossorbida 40%	17C29-B01-335071	1
Caelo	Dinitrato de isossorbida 40%	17c29-B01-339447	1
Caelo	Dinitrato de isossorbida 40%	17C29B01339447	1
Caelo	Dinitrato de isossorbida 40%	17C29-B01-339447	2
Caelo	Dinitrato de isossorbida 40%	17c29-b01-339448	1
Caelo	Dinitrato de isossorbida 40%	17C29-B01-347248	1
Caelo	Dinitrato de isossorbida 40%	17C29-B01-347589	3
Caelo	Dinitrato de isossorbida 40%	17c29-b01-347885	4
Caelo	Dinitrato de isossorbida 40%	17C29-B01-348859	2
Caelo	Dinitrato de isossorbida 40%	17C29-B01-348860	1
Caelo	Dinitrato de isossorbida 40%	17C29-B01-353161	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dinitrato de isossorbida 40%	18j18-b01-358247	1
Caelo	Dinitrato de isossorbida 40%	18J18-B01-363844	1
Caelo	Dinitrato de isossorbida 40%	18J18-B01-363845	1
Caelo	Dinitrato de isossorbida 40%	18J18-B01-373438	1
Caelo	Dinitrato de isossorbida 40%	193469	1
Caelo	Dinitrato de isossorbida 40%	195293	1
Caelo	Dinitrato de isossorbida 40%	701310-0001	1
Caelo	Dinitrato de isossorbida 40%	701319-0003	1
ebe a	Dinitrato de isossorbida 40%	14D09-B03-294281	1
Ebert-Jacobi	Dinitrato de isossorbida 40%	15I10-B01-328132	1
Euro OTC	Dinitrato de isossorbida 40%		1
Euro OTC	Dinitrato de isossorbida 40%	13126-N18	1
Euro OTC	Dinitrato de isossorbida 40%	15I10-B01325474	1
Euro OTC	Dinitrato de isossorbida 40%	22D11-B05-215487	1
Fagro/Noweda	Dinitrato de isossorbida 40%	17C29-B01-335070	1
Fagron	Dinitrato de isossorbida 40%		9
Fagron	Dinitrato de isossorbida 40%	10029-N10	1
Fagron	Dinitrato de isossorbida 40%	101652	6
Fagron	Dinitrato de isossorbida 40%	10-B01-320081	1
Fagron	Dinitrato de isossorbida 40%	10C19-N01	1
Fagron	Dinitrato de isossorbida 40%	10D29-N10	1
Fagron	Dinitrato de isossorbida 40%	11/17-N05	1
Fagron	Dinitrato de isossorbida 40%	11/17-No5	1
Fagron	Dinitrato de isossorbida 40%	11D12-N01	2
Fagron	Dinitrato de isossorbida 40%	11F28-N05	2
Fagron	Dinitrato de isossorbida 40%	11I17-N05	1
Fagron	Dinitrato de isossorbida 40%	11J17-N05	3
Fagron	Dinitrato de isossorbida 40%	11l17-N05	1
Fagron	Dinitrato de isossorbida 40%	1216M-03516	1
Fagron	Dinitrato de isossorbida 40%	12C08-N05	2
Fagron	Dinitrato de isossorbida 40%	12f08-n04	1
Fagron	Dinitrato de isossorbida 40%	12F08-N04	8
Fagron	Dinitrato de isossorbida 40%	12k14-n02	1
Fagron	Dinitrato de isossorbida 40%	12K14N02	1
Fagron	Dinitrato de isossorbida 40%	12K14-N02	6
Fagron	Dinitrato de isossorbida 40%	13/26-N18	1
Fagron	Dinitrato de isossorbida 40%	1309210009	1
Fagron	Dinitrato de isossorbida 40%	1-36384005	1
Fagron	Dinitrato de isossorbida 40%	1373438	1
Fagron	Dinitrato de isossorbida 40%	13A07-0003	1
Fagron	Dinitrato de isossorbida 40%	13A07-N13	7
Fagron	Dinitrato de isossorbida 40%	13d15-n02	1
Fagron	Dinitrato de isossorbida 40%	13D15-N02	7
Fagron	Dinitrato de isossorbida 40%	13F27-N04	6
Fagron	Dinitrato de isossorbida 40%	13F27-N040234/1300	1
Fagron	Dinitrato de isossorbida 40%	13I26-N18	10
Fagron	Dinitrato de isossorbida 40%	149168	11
Fagron	Dinitrato de isossorbida 40%	14D09-B03	9
Fagron	Dinitrato de isossorbida 40%	14D09-B03_294280	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03_294282	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03_308419	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-294280	9
Fagron	Dinitrato de isossorbida 40%	14D09B03294281	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-294281	4
Fagron	Dinitrato de isossorbida 40%	14D09-B03-294282	5
Fagron	Dinitrato de isossorbida 40%	14D09-B03-294282Eber	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-29481	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-300234	14
Fagron	Dinitrato de isossorbida 40%	14-D09-B03-300234	1
Fagron	Dinitrato de isossorbida 40%	14D09B03300235	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dinitrato de isossorbida 40%	14D09-B03-300235	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-305633	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-307018	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-308419	17
Fagron	Dinitrato de isossorbida 40%	14d09-b03-313566	1
Fagron	Dinitrato de isossorbida 40%	14D09-B03-313566	3
Fagron	Dinitrato de isossorbida 40%	14D09-B3-308419	1
Fagron	Dinitrato de isossorbida 40%	15/10B01-315217	1
Fagron	Dinitrato de isossorbida 40%	15/10-B01-315217	8
Fagron	Dinitrato de isossorbida 40%	15/10-B01-318522	1
Fagron	Dinitrato de isossorbida 40%	15/10-B01-3200782	1
Fagron	Dinitrato de isossorbida 40%	15/10-B01-320081	12
Fagron	Dinitrato de isossorbida 40%	15/10-B01-320782	1
Fagron	Dinitrato de isossorbida 40%	15/10-B01-325474	5
Fagron	Dinitrato de isossorbida 40%	15/10-b01-328132	3
Fagron	Dinitrato de isossorbida 40%	15/10-B01-328132	2
Fagron	Dinitrato de isossorbida 40%	15/10-B01-328577	9
Fagron	Dinitrato de isossorbida 40%	15/10-B01-331286	5
Fagron	Dinitrato de isossorbida 40%	15/10-b01-331287	3
Fagron	Dinitrato de isossorbida 40%	15/10-B01-331287	1
Fagron	Dinitrato de isossorbida 40%	15/10-B10-331286	1
Fagron	Dinitrato de isossorbida 40%	15/10-BO1-325474	1
Fagron	Dinitrato de isossorbida 40%	1510-B01-315217	2
Fagron	Dinitrato de isossorbida 40%	15-10-b01-318522	1
Fagron	Dinitrato de isossorbida 40%	1510B01320081	1
Fagron	Dinitrato de isossorbida 40%	1510-B01320081	1
Fagron	Dinitrato de isossorbida 40%	1510-B01-320081	1
Fagron	Dinitrato de isossorbida 40%	1510B01325474	2
Fagron	Dinitrato de isossorbida 40%	1510-B01-325474	1
Fagron	Dinitrato de isossorbida 40%	1510-b01-325475	3
Fagron	Dinitrato de isossorbida 40%	15-10-b01-325475	1
Fagron	Dinitrato de isossorbida 40%	1510-b01-328132	1
Fagron	Dinitrato de isossorbida 40%	1510B01328577	1
Fagron	Dinitrato de isossorbida 40%	1510-B01-328577	2
Fagron	Dinitrato de isossorbida 40%	15-10-b01-331287	5
Fagron	Dinitrato de isossorbida 40%	151-b01-328132	2
Fagron	Dinitrato de isossorbida 40%	15I10-B01	9
Fagron	Dinitrato de isossorbida 40%	15I10-B01-310081	1
Fagron	Dinitrato de isossorbida 40%	15I10-B01-315217	2
Fagron	Dinitrato de isossorbida 40%	15I10-B01-318522	2
Fagron	Dinitrato de isossorbida 40%	15I10-B01-320081	5
Fagron	Dinitrato de isossorbida 40%	15I10-B01-320782	2
Fagron	Dinitrato de isossorbida 40%	15I10-B01-325474	7
Fagron	Dinitrato de isossorbida 40%	15I10-B01-328132	1
Fagron	Dinitrato de isossorbida 40%	15I10-B01-328577	5
Fagron	Dinitrato de isossorbida 40%	15I10B01331286	1
Fagron	Dinitrato de isossorbida 40%	15I10-B01-331286	3
Fagron	Dinitrato de isossorbida 40%	15l10-B01-320081	1
Fagron	Dinitrato de isossorbida 40%	15l10-B01-325474	1
Fagron	Dinitrato de isossorbida 40%	15L10B01325474	1
Fagron	Dinitrato de isossorbida 40%	15l10-B01-328577	1
Fagron	Dinitrato de isossorbida 40%	15l10-B01-331286	1
Fagron	Dinitrato de isossorbida 40%	160629I	1
Fagron	Dinitrato de isossorbida 40%	17C26-B01-347885	1
Fagron	Dinitrato de isossorbida 40%	17C29_B01_350469	1
Fagron	Dinitrato de isossorbida 40%	17C29-801-347885	1
Fagron	Dinitrato de isossorbida 40%	17c29-b01	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01	14
Fagron	Dinitrato de isossorbida 40%	17C29-B01_339447	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01_350469	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dinitrato de isossorbida 40%	17c29b01335070	1
Fagron	Dinitrato de isossorbida 40%	17c29-b01-335070	2
Fagron	Dinitrato de isossorbida 40%	17C29B01335070	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01335070	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-335070	18
Fagron	Dinitrato de isossorbida 40%	17c29-b01-335071	6
Fagron	Dinitrato de isossorbida 40%	17C29-B01-335071	3
Fagron	Dinitrato de isossorbida 40%	17C29B01339447	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-339447	19
Fagron	Dinitrato de isossorbida 40%	17c29-b01-339448	1
Fagron	Dinitrato de isossorbida 40%	17C29-b01-339448	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-339448	4
Fagron	Dinitrato de isossorbida 40%	17C29-B01-346333	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-347248	4
Fagron	Dinitrato de isossorbida 40%	17C29B01347589	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-347589	16
Fagron	Dinitrato de isossorbida 40%	17C29-B01-347885	1
Fagron	Dinitrato de isossorbida 40%	17c29-b01-348859	3
Fagron	Dinitrato de isossorbida 40%	17C29B01348859	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-348859	22
Fagron	Dinitrato de isossorbida 40%	17C29-B01-348860	2
Fagron	Dinitrato de isossorbida 40%	17C29-B01-34889	1
Fagron	Dinitrato de isossorbida 40%	17c29-b01-350469	1
Fagron	Dinitrato de isossorbida 40%	17C29B01350469	1
Fagron	Dinitrato de isossorbida 40%	17C29-B01-350469	19
Fagron	Dinitrato de isossorbida 40%	17C29-B01-350470	2
Fagron	Dinitrato de isossorbida 40%	17C29-B01-352558	4
Fagron	Dinitrato de isossorbida 40%	17C29-B01-353161	4
Fagron	Dinitrato de isossorbida 40%	17c29-B01-48859	1
Fagron	Dinitrato de isossorbida 40%	17C29-Bo1347589	1
Fagron	Dinitrato de isossorbida 40%	17c9-b01-347589	1
Fagron	Dinitrato de isossorbida 40%	17C-B01-347589	1
Fagron	Dinitrato de isossorbida 40%	17V29-B01-347589	1
Fagron	Dinitrato de isossorbida 40%	18/18-B01-358241	1
Fagron	Dinitrato de isossorbida 40%	18/18-B01-359177	2
Fagron	Dinitrato de isossorbida 40%	18/18-B01-359178	2
Fagron	Dinitrato de isossorbida 40%	18-18-b01-358242	2
Fagron	Dinitrato de isossorbida 40%	1818b01359178	5
Fagron	Dinitrato de isossorbida 40%	1818B01373439	1
Fagron	Dinitrato de isossorbida 40%	1818bo1373439	1
Fagron	Dinitrato de isossorbida 40%	18J118-B01-363844	1
Fagron	Dinitrato de isossorbida 40%	18J18_B01_358247	1
Fagron	Dinitrato de isossorbida 40%	18J18_B01_373439	1
Fagron	Dinitrato de isossorbida 40%	18J18-01-370272	1
Fagron	Dinitrato de isossorbida 40%	18J18-01-373438	1
Fagron	Dinitrato de isossorbida 40%	18j18-B01	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01	20
Fagron	Dinitrato de isossorbida 40%	18J18-B01-258241	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-263844	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-3395177	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-358241	25
Fagron	Dinitrato de isossorbida 40%	18J18B01358242	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-358242	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-358247	16
Fagron	Dinitrato de isossorbida 40%	18j18-b01-359177	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01359177	2
Fagron	Dinitrato de isossorbida 40%	18J18-B01-359177	38
Fagron	Dinitrato de isossorbida 40%	18J-18-B01-359177	1
Fagron	Dinitrato de isossorbida 40%	18J18B01359178	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-359178	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dinitrato de isossorbida 40%	18J18-B01359579	1
Fagron	Dinitrato de isossorbida 40%	18J18B01361397	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-3638345	1
Fagron	Dinitrato de isossorbida 40%	18J18-b01-363844	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-363844	24
Fagron	Dinitrato de isossorbida 40%	18j18-b01-363845	1
Fagron	Dinitrato de isossorbida 40%	18J18B01363845	1
Fagron	Dinitrato de isossorbida 40%	18J18B01-363845	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-363845	26
Fagron	Dinitrato de isossorbida 40%	18j18-b01-363846	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-363846	5
Fagron	Dinitrato de isossorbida 40%	18J18B01365264	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-3702702	1
Fagron	Dinitrato de isossorbida 40%	18j18-b01-370272	1
Fagron	Dinitrato de isossorbida 40%	18J18B01370272	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-370272	38
Fagron	Dinitrato de isossorbida 40%	18J18b01373438	1
Fagron	Dinitrato de isossorbida 40%	18J18B01-373438	1
Fagron	Dinitrato de isossorbida 40%	18J18-B01-373438	12
Fagron	Dinitrato de isossorbida 40%	18J18-B01-373439	2
Fagron	Dinitrato de isossorbida 40%	18J18-BO1-359177	1
Fagron	Dinitrato de isossorbida 40%	18J18-BO1-3702702	1
Fagron	Dinitrato de isossorbida 40%	18J18-BO1-373438	2
Fagron	Dinitrato de isossorbida 40%	18J19-B01	1
Fagron	Dinitrato de isossorbida 40%	1934469	1
Fagron	Dinitrato de isossorbida 40%	193469	12
Fagron	Dinitrato de isossorbida 40%	195293	26
Fagron	Dinitrato de isossorbida 40%	2114M3516	1
Fagron	Dinitrato de isossorbida 40%	2203089	6
Fagron	Dinitrato de isossorbida 40%	22D11-B05-215487	11
Fagron	Dinitrato de isossorbida 40%	22D11-B05-215525	8
Fagron	Dinitrato de isossorbida 40%	22D11-B05-216314	13
Fagron	Dinitrato de isossorbida 40%	22D11-B05-216315	1
Fagron	Dinitrato de isossorbida 40%	22D11-B05-225756	1
Fagron	Dinitrato de isossorbida 40%	22D11-B05-225757	2
Fagron	Dinitrato de isossorbida 40%	22D11-BO5	1
Fagron	Dinitrato de isossorbida 40%	2413Q03516	1
Fagron	Dinitrato de isossorbida 40%	25021711	1
Fagron	Dinitrato de isossorbida 40%	2817E-03516	1
Fagron	Dinitrato de isossorbida 40%	3115M-03516	1
Fagron	Dinitrato de isossorbida 40%	3211U-03516	1
Fagron	Dinitrato de isossorbida 40%	3413U03516	1
Fagron	Dinitrato de isossorbida 40%	3518M-03516	1
Fagron	Dinitrato de isossorbida 40%	359177	2
Fagron	Dinitrato de isossorbida 40%	391311-03516	1
Fagron	Dinitrato de isossorbida 40%	4314U-03516	1
Fagron	Dinitrato de isossorbida 40%	517I-03516	1
Fagron	Dinitrato de isossorbida 40%	701319-0001	1
Fagron	Dinitrato de isossorbida 40%	7013190003	1
Fagron	Dinitrato de isossorbida 40%	8564340	1
Fagron	Dinitrato de isossorbida 40%	9101205	1
Fagron	Dinitrato de isossorbida 40%	9E05-N05	1
Fagron	Dinitrato de isossorbida 40%	B01-3591707	2
Fagron	Dinitrato de isossorbida 40%	B01-3591708	1
Fagron	Dinitrato de isossorbida 40%	B01-3638404	8
Fagron	Dinitrato de isossorbida 40%	B01-3638406	2
Fagron	Dinitrato de isossorbida 40%	B01-363844	1
Fagron	Dinitrato de isossorbida 40%	B01-3702702	10
Fagron	Dinitrato de isossorbida 40%	B01-3734308	2
Fagron	Dinitrato de isossorbida 40%	B013734309	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dinitrato de isossorbida 40%	B01-3734309	1
Fagron	Dinitrato de isossorbida 40%	B05-2154807	1
Fagron	Dinitrato de isossorbida 40%	B05-2163104	1
Fagron	Dinitrato de isossorbida 40%	IN20012021	1
Fagron	Dinitrato de isossorbida 40%	P11008	1
Fagron	Dinitrato de isossorbida 40%	testxx	1
Fagron	Dinitrato de isossorbida 40%	X12010	1
Fargon / AHD	Dinitrato de isossorbida 40%	18J18-B01-363844	1
Fargon/Gehe	Dinitrato de isossorbida 40%	15/10-B01-331286	1
Fargon/Gehe	Dinitrato de isossorbida 40%	17C29-B01-339447	1
Fargon/Gehe	Dinitrato de isossorbida 40%	17C29-B01-348859	1
Fargon/Gehe	Dinitrato de isossorbida 40%	18J18-B01-373438	1
Fargon/Noweda	Dinitrato de isossorbida 40%	18j18-B01-359177	1
Fargon/Spangro	Dinitrato de isossorbida 40%	195293	1
Fargon	Dinitrato de isossorbida 40%	15/10-B01-320081	1
Fargon	Dinitrato de isossorbida 40%	17C29-B01	1
Fargon	Dinitrato de isossorbida 40%	18J18-B01	3
Fargon	Dinitrato de isossorbida 40%	18J18-B01-363845	1
Fargron / Gehe	Dinitrato de isossorbida 40%	17C29-B01-339447	1
Fiebig 23.05.13 ek: ...	Dinitrato de isossorbida 40%	12F08-N04	1
Fiebig	Dinitrato de isossorbida 40%	17C29-B01-350469	1
Fiebig	Dinitrato de isossorbida 40%	18j18-b01-358247	1
Fiebig	Dinitrato de isossorbida 40%	18J18-B01-359177	1
Fiebig	Dinitrato de isossorbida 40%	18J18-B01-363844	1
Fiebig	Dinitrato de isossorbida 40%	18J18-B01-363846	1
Fiebig	Dinitrato de isossorbida 40%	bo1-3702702	1
Fischar/Allia	Dinitrato de isossorbida 40%	18J18-B01-358241	2
Frago/Gehe	Dinitrato de isossorbida 40%	17C29-B01-335070	1
Frago/Noweda	Dinitrato de isossorbida 40%	15I10-B01-328577	1
Gehe amax	Dinitrato de isossorbida 40%	15I10-B01-331286	1
Gehe amax	Dinitrato de isossorbida 40%	18J18-B01-363844	1
Gehe amax	Dinitrato de isossorbida 40%	18J18-B01-363845	2
Gehe amax	Dinitrato de isossorbida 40%	18J18-B01-370272	1
Gehe	Dinitrato de isossorbida 40%	17c29-B01-335070	1
GEHE	Dinitrato de isossorbida 40%	17C29-B01-347589	1
Gehe	Dinitrato de isossorbida 40%	18J18-B01	1
Gehe	Dinitrato de isossorbida 40%	18J18-B01-358241	1
Gehe	Dinitrato de isossorbida 40%	18J18-B01-358247	1
Gehe	Dinitrato de isossorbida 40%	18J18-B01-373438	1
Gehe	Dinitrato de isossorbida 40%	22D11-B05-216314	1
Gehe	Dinitrato de isossorbida 40%	22D11-B05-225756	1
Gehe	Dinitrato de isossorbida 40%	B01-3702702	1
Ichthyol-Gesellschaft	Dinitrato de isossorbida 40%	17C29-B01-335070	1
Kehr	Dinitrato de isossorbida 40%	200051401	1
Kehr	Dinitrato de isossorbida 40%	22D11-B05-216314	1
Krieger	Dinitrato de isossorbida 40%	3186	1
L12	Dinitrato de isossorbida 40%	149168	1
L12	Dinitrato de isossorbida 40%	15I10-B01-331286	2
Noweda / Fargon	Dinitrato de isossorbida 40%	18j18-B01	1
Noweda	Dinitrato de isossorbida 40%	15/10-B01-315217	1
Noweda	Dinitrato de isossorbida 40%	15I10-B01-331287	1
Noweda	Dinitrato de isossorbida 40%	17C29-B01-350469	1
Noweda	Dinitrato de isossorbida 40%	17C29-B01-352558	1
Noweda	Dinitrato de isossorbida 40%	195293	1
Noweda	Dinitrato de isossorbida 40%	22D11-B05-225756	2
Phoenix	Dinitrato de isossorbida 40%	3066	1
Phoenix	Dinitrato de isossorbida 40%	3362	1
Phönix	Dinitrato de isossorbida 40%	13A07-N13	1
Sanacorp	Dinitrato de isossorbida 40%	11J17-N05	1
Sanacorp	Dinitrato de isossorbida 40%	14D09-B03-294280	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Dinitrato de isossorbida 40%	18J18-B01-358241	1
Sanacorp	Dinitrato de isossorbida 40%	18J18-B01-358247	2
Sanacorp	Dinitrato de isossorbida 40%	18J18-B01-359177	1
Sanacorp	Dinitrato de isossorbida 40%	18J18-B01-363845	1
Sanacorp	Dinitrato de isossorbida 40%	18J18-B01-363846	1
Sanacorp	Dinitrato de isossorbida 40%	193469	1
Sanacorp	Dinitrato de isossorbida 40%	22d11-b05-215525	1
Sanacorp	Dinitrato de isossorbida 40%	22D11-B05-216314	1
Sanacorp	Dinitrato de isossorbida 40%	22D11-B05-229443	2
UCB manufacturing Ireland	Dinitrato de isossorbida 40%	14D09-B03-300234	2
VDl 28.10.14 10,32 euro	Dinitrato de isossorbida 40%		1
VDL	Dinitrato de isossorbida 40%	18J18-B01-358247	1
Wepa	Dinitrato de isossorbida 40%	14D09-B03-313566	1

- 235 013 spectra from 1515 *Apo-Ident* customers from a total of 48 990 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dinitrato de isossorbida 40%* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dinitrato de isossorbida 40%* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	229	0	152 733
Type B	0	150	0	201 934
Type C	0	1040	14	235 013

The substance/substance group *Dinitrato de isossorbida 40%* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.3799 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.6717 % (> 98.3871 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20891	23200	14,42	189,73
21347	23200	7,55	190,76
23200	23200	0,00	184,45
23598	23200	8,21	185,41
24057	23200	10,35	182,71
27044	23200	8,23	177,66

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diosmina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006687-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diosmina

Special notes

When selecting the *Diosmina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diosmina	2	1	0

Second-stage model

For differentiation of the substance/substance group *Diosmina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diosmina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	61,58	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diosmina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diosmina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Diosmina	DSM240602	BR20038	40	20241031*
Fagron	Diosmina	DSM240401	BR20039	40	20241031*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Diosmina*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 4 reference samples from the substance/substance group *Diosmina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Diosmina	DSM240603	BR20040	40
Fagron	Diosmina	DSM240602	BR20038SI†	20
Fagron	Diosmina	DSM240401	BR20039SI†	20
Fagron	Diosmina	DSM240603	BR20040SI	20

- 201 984 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Diosmina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diosmina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

relevant spectra of the various substances were compared with *Diosmina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	100	0	201 984
Type C	0	0	0	236 067

The substance/substance group *Diosmina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
BR20038	BR20038	0,00	84,20
BR20039	BR20039	0,00	81,30

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dipropionato de beclometasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21046-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dipropionato de beclometasona; Beclometasona, dipropionato; Beclometasoni dipropionas

Special notes

When selecting the *Dipropionato de beclometasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dipropionato de beclometasona	6	4	43

Second-stage model

For differentiation of the substance/substance group *Dipropionato de beclometasona* the following second-stage model is used:

- Submodelo 15

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dipropionato de beclometasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Propionato de clobetasol	52,96	58,11
⋮	⋮	⋮
Dipropionato de betametasona	>50	33,20

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dipropionato de beclometasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dipropionato de beclometasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Dipropionato de beclometasona	1203022-03	21634	55	1509281
Euro OTC	Dipropionato de beclometasona	1203022-03	21995	60	20120424
Euro OTC	Dipropionato de beclometasona	1502032	22989	40	20150327*
Euro OTC	Dipropionato de beclometasona	1502032	22989SI	30	20150327*
Euro OTC	Dipropionato de beclometasona	1502032	24869	40	20190828*
Fagron	Dipropionato de beclometasona	13I05-N03	21046	60	1511689
Fagron	Dipropionato de beclometasona	13E02-B40-293328	21554	40	20140508
Fagron	Dipropionato de beclometasona	13E02-B40-296353	21977	60	20140508
Fagron	Dipropionato de beclometasona	13E02-B40-296353	21977SI	29	20140508
Fagron	Dipropionato de beclometasona	20C17-F03-376057	25743	40	20200518
Fagron	Dipropionato de beclometasona	20C17-F03-376057	25743SI	32	20200518

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 486 spectra of 11 reference samples from the substance/substance group *Dipropionato de beclometasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 476 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 359 spectra of 11 reference samples from the substance/substance group *Dipropionato de beclometasona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Dipropionato de beclometasona	15F29-B09-314376	23104	40
Fagron	Dipropionato de beclometasona	16B16-B03-342082	23930	40
Fagron	Dipropionato de beclometasona	19J02-F03-374146	25717	50
Fagron	Dipropionato de beclometasona	21K15-B03-230979	27177	40
Euro OTC	Dipropionato de beclometasona	1203022-03	21634†	5
Euro OTC	Dipropionato de beclometasona	1203022-03	21995SI†	28
Euro OTC	Dipropionato de beclometasona	1502032	24869SI†	31
Fagron	Dipropionato de beclometasona	15F29-B09-314376	23104SI	20
Fagron	Dipropionato de beclometasona	16B16-B03-342082	23930SI	25
Fagron	Dipropionato de beclometasona	19J02-F03-374146	25717SI	40
Fagron	Dipropionato de beclometasona	21K15-B03-230979	27177SI	40

- 201 725 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 87 spectra from 35 *Apo-Ident* customers from 48 batches from the substance/substance group *Dipropionato de beclometasona*.
- Among them are spectra of independent samples from 42 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Dipropionato de beclometasona	13E02-B40-293326	1
Caelo	Dipropionato de beclometasona	18c05b01358707	1
Caelo	Dipropionato de beclometasona	21K15-B03-213640	1
Euro OTC	Dipropionato de beclometasona	1203022-01	2
Euro OTC	Dipropionato de beclometasona	1203022-03	1
Euro OTC	Dipropionato de beclometasona	1502032	1
Euro OTC	Dipropionato de beclometasona	1502032-01	1
Euro OTC	Dipropionato de beclometasona	1502032-02	3
Euro OTC	Dipropionato de beclometasona	1502032-03	2
Euro OTC	Dipropionato de beclometasona	18041820	1
Euro OTC	Dipropionato de beclometasona	C0783111020	1
Fagro/Noweda	Dipropionato de beclometasona	14D04-B04-302335	1
Fagron	Dipropionato de beclometasona		1
Fagron	Dipropionato de beclometasona	11F28-N02	2
Fagron	Dipropionato de beclometasona	11L01-N03	1
Fagron	Dipropionato de beclometasona	12D12-N03	4
Fagron	Dipropionato de beclometasona	12G04-N11	3
Fagron	Dipropionato de beclometasona	13/05-N03	1
Fagron	Dipropionato de beclometasona	13/05-N03	1
Fagron	Dipropionato de beclometasona	13E02-B40	1
Fagron	Dipropionato de beclometasona	13E02-B40-293327	4
Fagron	Dipropionato de beclometasona	13E02-B40-293328	2
Fagron	Dipropionato de beclometasona	13E02-B40-296353	1
Fagron	Dipropionato de beclometasona	13E02-B40-296354	2
Fagron	Dipropionato de beclometasona	13I05N03	1
Fagron	Dipropionato de beclometasona	13I05-N03	3
Fagron	Dipropionato de beclometasona	14D04-B04-302335	1
Fagron	Dipropionato de beclometasona	14D04-B04302336	1
Fagron	Dipropionato de beclometasona	14D04-B04-302336	3
Fagron	Dipropionato de beclometasona	15F29-B09-314376	1
Fagron	Dipropionato de beclometasona	16B16-B03-318877	3
Fagron	Dipropionato de beclometasona	16B16-B03-322517	2
Fagron	Dipropionato de beclometasona	16B16-B03-333670	2
Fagron	Dipropionato de beclometasona	16B16-B03-342082	1
Fagron	Dipropionato de beclometasona	18C05-B01-347367	3
Fagron	Dipropionato de beclometasona	18C05-B01-347369	5
Fagron	Dipropionato de beclometasona	18C05-B01-351434	2
Fagron	Dipropionato de beclometasona	18C05-B01-358708	1
Fagron	Dipropionato de beclometasona	19J02-F03	3
Fagron	Dipropionato de beclometasona	19j02f03365514	2
Fagron	Dipropionato de beclometasona	19J02-F03-365513	1
Fagron	Dipropionato de beclometasona	21K15-B03-213638	5
Fagron	Dipropionato de beclometasona	21k15b03213639	1
Fagron	Dipropionato de beclometasona	21K15-B03-226133	1
Fagron	Dipropionato de beclometasona	BMD/M/021/19	1
Fagron	Dipropionato de beclometasona	C0783/112020	1
Fagron	Dipropionato de beclometasona	F03-3741405	2
Fagron	Dipropionato de beclometasona	P-26061721/322517	1
fragon	Dipropionato de beclometasona	700721-0004	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 980 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dipropionato de beclometasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dipropionato de beclometasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	486	0	152 476
Type B	0	359	0	201 725
Type C	0	85	2	235 980

The substance/substance group *Dipropionato de beclometasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7654 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3287 %)
Type C	100.0000 % (> 99.9007 %)	97.7011 % (> 94.2529 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21046	21046	0,00	63,83
21554	21634	5,22	57,29
21634	21634	0,00	57,37
21977	24869	5,05	61,76
21995	24869	6,98	62,26
22989	22989	0,00	60,33
24869	24869	0,00	60,61
25743	24869	5,42	62,30

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dipropionato de betametasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20930-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dipropionato de betametasona; Betametasona, dipropionato; Betamethasoni dipropionas

Special notes

When selecting the *Dipropionato de betametasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dipropionato de betametasona	7	14	284

Second-stage model

For differentiation of the substance/substance group *Dipropionato de betametasona* the following second-stage model is used:

- Submodelo 15

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dipropionato de betametasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dipropionato de beclometasona	37,10	33,36
Propionato de clobetasol	38,35	53,00

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dipropionato de betametasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dipropionato de betametasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dipropionato de betametasona	13372501	21250	40	AR-15-FG-005428-01
Caelo	Dipropionato de betametasona	13236803	21366	50	20130730
Caelo	Dipropionato de betametasona	13236803	21367	40	20130730
Euro OTC	Dipropionato de betametasona	1311023-01	21716	60	1505455
Euro OTC	Dipropionato de betametasona	1601034	22372	45	20160204*
Euro OTC	Dipropionato de betametasona	2102001	25691	50	20210528*
Euro OTC	Dipropionato de betametasona	2102001	25691SI	50	20210528*
Fagron	Dipropionato de betametasona	13I17-N05	20930	40	1401377
Fagron	Dipropionato de betametasona	13I17-N05	20952	80	20130926
Fagron	Dipropionato de betametasona	16C04-B03-324513	22898	40	20160421
Fagron	Dipropionato de betametasona	16C04-B03-324513	22898SI	39	20160421

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 534 spectra of 11 reference samples from the substance/substance group *Dipropionato de betametasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 428 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1293 spectra of 33 reference samples from the substance/substance group *Dipropionato de betametasona*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dipropionato de betametasona	171059	23342	40
Caelo	Dipropionato de betametasona	173536	23839	40
Caelo	Dipropionato de betametasona	22001649001	26313	40
Euro OTC	Dipropionato de betametasona	1610014	22851	40
Euro OTC	Dipropionato de betametasona	1705020	23539	40
Euro OTC	Dipropionato de betametasona	1801045	24090	40
Euro OTC	Dipropionato de betametasona	1811007	24343	40
Euro OTC	Dipropionato de betametasona	1907034	24796	40
Euro OTC	Dipropionato de betametasona	2003057	25309	40
Euro OTC	Dipropionato de betametasona	2110005	25914	40
Euro OTC	Dipropionato de betametasona	2208030	26345	40
Euro OTC	Dipropionato de betametasona	2301013	26573	40
Euro OTC	Dipropionato de betametasona	2406016	27350	40
Fagron	Dipropionato de betametasona	21K24-B04-216140	26178	40
Caelo	Dipropionato de betametasona	13372501	21250SI†	45
Caelo	Dipropionato de betametasona	13236803	21366SI†	46
Caelo	Dipropionato de betametasona	13236803	21367SI†	60
Caelo	Dipropionato de betametasona	171059	23342SI	20
Caelo	Dipropionato de betametasona	173536	23839SI	25
Caelo	Dipropionato de betametasona	22001649001	26313SI	40
Euro OTC	Dipropionato de betametasona	1311023-01	21716SI†	46
Euro OTC	Dipropionato de betametasona	1601034	22372SI†	45

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Dipropionato de betametasona	1610014	22851SI	30
Euro OTC	Dipropionato de betametasona	1705020	23539SI	27
Euro OTC	Dipropionato de betametasona	1801045	24090SI	39
Euro OTC	Dipropionato de betametasona	1811007	24343SI	30
Euro OTC	Dipropionato de betametasona	1907034	24796SI	40
Euro OTC	Dipropionato de betametasona	2003057	25309SI	40
Euro OTC	Dipropionato de betametasona	2110005	25914SI	40
Euro OTC	Dipropionato de betametasona	2208030	26345SI	40
Euro OTC	Dipropionato de betametasona	2301013	26573SI	40
Euro OTC	Dipropionato de betametasona	2406016	27350SI	40
Fagron	Dipropionato de betametasona	21K24-B04-216140	26178SI	40

- 200 791 spectra from a total of 4027 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1624 spectra from 648 *Apo-Ident* customers from 302 batches from the substance/substance group *Dipropionato de betametasona*.

- Among them are spectra of independent samples from 284 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dipropionato de betametasona		1
	Dipropionato de betametasona	13/17-N05	2
	Dipropionato de betametasona	2110005-01	1
	Dipropionato de betametasona	21H18-B04-213656	1
	Dipropionato de betametasona	21K24-B04-220120	1
	Dipropionato de betametasona	21K24-B04-227289	1
	Dipropionato de betametasona	21K24-B04-227290	1
	Dipropionato de betametasona	22001649003	1
	Dipropionato de betametasona	22001649007	4
	Dipropionato de betametasona	22001649008	5
	Dipropionato de betametasona	22001649009	2
	Dipropionato de betametasona	22003962001	2
	Dipropionato de betametasona	22003962002	8
	Dipropionato de betametasona	2208030-01	7
	Dipropionato de betametasona	228030-01	1
	Dipropionato de betametasona	2301013-01	2
AHD/Caesar & Loretz GmbH	Dipropionato de betametasona	21000648013	1
AHD	Dipropionato de betametasona	18B06-B05-346219	1
Alliance Health 24.0...	Dipropionato de betametasona	13/17-N05	1
Alliance	Dipropionato de betametasona	22003962001	2
Anzag	Dipropionato de betametasona	12114513	2
Bombastus	Dipropionato de betametasona	12B27N08	1
cae	Dipropionato de betametasona	17353601	1
Cae	Dipropionato de betametasona	18293408	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dipropionato de betametasona		2
Caelo	Dipropionato de betametasona	1210020-01	1
Caelo	Dipropionato de betametasona	12114501	1
Caelo	Dipropionato de betametasona	12114506	1
Caelo	Dipropionato de betametasona	12114507	2
Caelo	Dipropionato de betametasona	12114511	2
Caelo	Dipropionato de betametasona	12114512	1
Caelo	Dipropionato de betametasona	12114513	1
Caelo	Dipropionato de betametasona	13/17-N05	2
Caelo	Dipropionato de betametasona	13023001	3
Caelo	Dipropionato de betametasona	13023002	5
Caelo	Dipropionato de betametasona	13023002NP	1
Caelo	Dipropionato de betametasona	13023005	7
Caelo	Dipropionato de betametasona	1303006-01	1
Caelo	Dipropionato de betametasona	13125701	3
Caelo	Dipropionato de betametasona	13125703	5
Caelo	Dipropionato de betametasona	13236801	6
Caelo	Dipropionato de betametasona	13236801ok	1
Caelo	Dipropionato de betametasona	13236802	4
Caelo	Dipropionato de betametasona	13236803	1
Caelo	Dipropionato de betametasona	13236805	5
Caelo	Dipropionato de betametasona	13236806	3
Caelo	Dipropionato de betametasona	1325702	1
Caelo	Dipropionato de betametasona	13372501	3
Caelo	Dipropionato de betametasona	13372503	7
Caelo	Dipropionato de betametasona	13372504	5
Caelo	Dipropionato de betametasona	13372512	1
Caelo	Dipropionato de betametasona	13372514	12
Caelo	Dipropionato de betametasona	13372515	3
Caelo	Dipropionato de betametasona	13372516	4
Caelo	Dipropionato de betametasona	13372520	2
Caelo	Dipropionato de betametasona	140507	1
Caelo	Dipropionato de betametasona	14C03-B06-296837	1
Caelo	Dipropionato de betametasona	1503003-01	2
Caelo	Dipropionato de betametasona	1503003-02	1
Caelo	Dipropionato de betametasona	150605BD	1
Caelo	Dipropionato de betametasona	15163204	1
Caelo	Dipropionato de betametasona	15163301	15
Caelo	Dipropionato de betametasona	15163302	6
Caelo	Dipropionato de betametasona	15163303	12
Caelo	Dipropionato de betametasona	15163304	14
Caelo	Dipropionato de betametasona	15163305	1
Caelo	Dipropionato de betametasona	15238701	32
Caelo	Dipropionato de betametasona	15412901	1
Caelo	Dipropionato de betametasona	15412903	2
Caelo	Dipropionato de betametasona	15412905	1
Caelo	Dipropionato de betametasona	15412906	12
Caelo	Dipropionato de betametasona	15412907	5
Caelo	Dipropionato de betametasona	15412909	1
Caelo	Dipropionato de betametasona	15412910	7
Caelo	Dipropionato de betametasona	15412913	1
Caelo	Dipropionato de betametasona	15412914	7
Caelo	Dipropionato de betametasona	15412915	2
Caelo	Dipropionato de betametasona	15412916	1
Caelo	Dipropionato de betametasona	15H28-B06	1
Caelo	Dipropionato de betametasona	15H28B06313088	1
Caelo	Dipropionato de betametasona	15H28-B06-313088	1
Caelo	Dipropionato de betametasona	15-H28-B06-313088	1
Caelo	Dipropionato de betametasona	17015905	1
Caelo	Dipropionato de betametasona	1705020-01	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dipropionato de betametasona	17105901	19
Caelo	Dipropionato de betametasona	17105902	17
Caelo	Dipropionato de betametasona	17105903	1
Caelo	Dipropionato de betametasona	17105905	4
Caelo	Dipropionato de betametasona	17105906	16
Caelo	Dipropionato de betametasona	17105907	10
Caelo	Dipropionato de betametasona	17105909	3
Caelo	Dipropionato de betametasona	17105911	6
Caelo	Dipropionato de betametasona	17353601	20
Caelo	Dipropionato de betametasona	17353603	16
Caelo	Dipropionato de betametasona	1735601	1
Caelo	Dipropionato de betametasona	17B16-B04	1
Caelo	Dipropionato de betametasona	17B16-B04-332220	1
Caelo	Dipropionato de betametasona	17E22-B06-336993	1
Caelo	Dipropionato de betametasona	17H16B04340537	1
Caelo	Dipropionato de betametasona	1801045-01	3
Caelo	Dipropionato de betametasona	18041819	1
Caelo	Dipropionato de betametasona	18090601	7
Caelo	Dipropionato de betametasona	18090602	7
Caelo	Dipropionato de betametasona	18090603	13
Caelo	Dipropionato de betametasona	18090606	22
Caelo	Dipropionato de betametasona	18090607	14
Caelo	Dipropionato de betametasona	18090608	15
Caelo	Dipropionato de betametasona	1811007-01	2
Caelo	Dipropionato de betametasona	18121306	1
Caelo	Dipropionato de betametasona	18292406	1
Caelo	Dipropionato de betametasona	18293402	12
Caelo	Dipropionato de betametasona	18293404	14
Caelo	Dipropionato de betametasona	182934046	1
Caelo	Dipropionato de betametasona	18293406	26
Caelo	Dipropionato de betametasona	18293407	4
Caelo	Dipropionato de betametasona	18293408	26
Caelo	Dipropionato de betametasona	18294306	1
Caelo	Dipropionato de betametasona	18B06-B05-350473	2
Caelo	Dipropionato de betametasona	18B06-B05-352731	1
Caelo	Dipropionato de betametasona	19000537003	10
Caelo	Dipropionato de betametasona	19000537007	24
Caelo	Dipropionato de betametasona	19000537008	5
Caelo	Dipropionato de betametasona	19000537010	10
Caelo	Dipropionato de betametasona	1900537008	1
Caelo	Dipropionato de betametasona	1900537010	1
Caelo	Dipropionato de betametasona	1907034-01	1
Caelo	Dipropionato de betametasona	20003997001	7
Caelo	Dipropionato de betametasona	20003997002	8
Caelo	Dipropionato de betametasona	20003997005	14
Caelo	Dipropionato de betametasona	2000648010	1
Caelo	Dipropionato de betametasona	21000645001	2
Caelo	Dipropionato de betametasona	21000648001	1
Caelo	Dipropionato de betametasona	21000648002	4
Caelo	Dipropionato de betametasona	21000648003	5
Caelo	Dipropionato de betametasona	21000648004	5
Caelo	Dipropionato de betametasona	21000648006	3
Caelo	Dipropionato de betametasona	21000648007	11
Caelo	Dipropionato de betametasona	21000648010	10
Caelo	Dipropionato de betametasona	21000648012	2
Caelo	Dipropionato de betametasona	21000648013	8
Caelo	Dipropionato de betametasona	21000648014	4
Caelo	Dipropionato de betametasona	2100648006	1
Caelo	Dipropionato de betametasona	2109DMOB00111322	1
Caelo	Dipropionato de betametasona	21648004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dipropionato de betametasona	22001649001	13
Caelo	Dipropionato de betametasona	22001649002	10
Caelo	Dipropionato de betametasona	22001649003	1
Caelo	Dipropionato de betametasona	22001649005	3
Caelo	Dipropionato de betametasona	22001649007	2
Caelo	Dipropionato de betametasona	22001649008	1
Caelo	Dipropionato de betametasona	22003962002	1
Caelo	Dipropionato de betametasona	220621(21000648014)	1
Caelo	Dipropionato de betametasona	3170717	1
Caelo	Dipropionato de betametasona	700216-0001	1
Caelo	Dipropionato de betametasona	8K03-N13	1
Caelo	Dipropionato de betametasona	AKD11	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18293406	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18293402	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18293408	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18090603	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	22001649005	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18293408	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	22001649005	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	21000648013	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	21000648007	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	19000537003	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18293408	1
Caesar & Loretz GmbH/Gehe	Dipropionato de betametasona	18090606	2
Caesar & Loretz GmbH/Gehe	Dipropionato de betametasona	19000537003	1
Caesar & Loretz GmbH/Gehe	Dipropionato de betametasona	20003997001	1
Caesar & Loretz GmbH/Gehe	Dipropionato de betametasona	21000648006	2
Caesar & Loretz GmbH/Gehe	Dipropionato de betametasona	21000648010	1
Caesar & Loretz GmbH/K	Dipropionato de betametasona	21000648013	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18090602	2
Caesar & Loretz GmbH...	Dipropionato de betametasona	19000537010	2
Caesar & Loretz GmbH...	Dipropionato de betametasona	20003997005	2
Caesar & Loretz GmbH...	Dipropionato de betametasona	20003997002	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	21000648004	1
Caesar & Loretz GmbH/S	Dipropionato de betametasona	21000648007	1
Caesar & Loretz GmbH/S	Dipropionato de betametasona	22001649002	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	18293406	3
Caesar & Loretz GmbH...	Dipropionato de betametasona	21000648007	1
Caesar & Loretz GmbH...	Dipropionato de betametasona	21000648014	1
Caesar & Loretz GmbH	Dipropionato de betametasona	17105902	1
Caesar & Loretz GmbH	Dipropionato de betametasona	17353605	1
Caesar & Loretz GmbH	Dipropionato de betametasona	18090606	2
Caesar & Loretz GmbH	Dipropionato de betametasona	18090608	1
Caesar & Loretz GmbH	Dipropionato de betametasona	18293402	3
Caesar & Loretz GmbH	Dipropionato de betametasona	18293404	5
Caesar & Loretz GmbH	Dipropionato de betametasona	18293406	8
Caesar & Loretz GmbH	Dipropionato de betametasona	18293407	1
Caesar & Loretz GmbH	Dipropionato de betametasona	18293408	7
Caesar & Loretz GmbH	Dipropionato de betametasona	19000537003	4
Caesar & Loretz GmbH	Dipropionato de betametasona	19000537007	6
Caesar & Loretz GmbH	Dipropionato de betametasona	19000537008	2
Caesar & Loretz GmbH	Dipropionato de betametasona	19000537010	1
Caesar & Loretz GmbH	Dipropionato de betametasona	20003997001	5
Caesar & Loretz GmbH	Dipropionato de betametasona	20003997002	3
Caesar & Loretz GmbH	Dipropionato de betametasona	20003997005	11
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648001	2
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648002	7
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648003	3
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648004	4
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648006	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648007	2
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648010	3
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648012	3
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648013	2
Caesar & Loretz GmbH	Dipropionato de betametasona	21000648014	2
Caesar & Loretz GmbH	Dipropionato de betametasona	22001649001	6
Caesar & Loretz GmbH	Dipropionato de betametasona	22001649002	3
Caesar & Loretz Hild...	Dipropionato de betametasona	18293408	1
Caesar & Loretz Hilden	Dipropionato de betametasona	18293404	1
Caesar & Loretz Hilden	Dipropionato de betametasona	18293406	1
Caesar & Loretz Hilden	Dipropionato de betametasona	19000537007	1
Caesar & Loretz	Dipropionato de betametasona	22001649002	1
Caesar & Loretz	Dipropionato de betametasona	22001649005	1
Cealo / Otto Geilenk...	Dipropionato de betametasona	18293402	1
Cealo/ AHD	Dipropionato de betametasona	18293402	1
Cealo/Sanacorp	Dipropionato de betametasona	13125701	1
Cealo	Dipropionato de betametasona	17353601	1
Crystal Pharma / Ebert	Dipropionato de betametasona	15163301	1
Crystal Pharma / Gehe	Dipropionato de betametasona	17105906	1
Delta	Dipropionato de betametasona	18B06-B05-346219	1
EU RHO/GEHE	Dipropionato de betametasona	2003057-01	1
EuRho/ Noweda	Dipropionato de betametasona	2003057-01	1
EuRho/ Noweda	Dipropionato de betametasona	2208030-01	1
EuRho/Alliance	Dipropionato de betametasona	2003057-01	1
EuRho/Fiebig	Dipropionato de betametasona	1811007-01	1
EuRho/Noweda	Dipropionato de betametasona	1907034-01	2
EuRho/Phoenix	Dipropionato de betametasona	2102001-01	1
Eurho/Phönix	Dipropionato de betametasona		1
EuRho/Phönix	Dipropionato de betametasona	2003057-01	1
euro AHD	Dipropionato de betametasona	1801045-015715	1
euro AHD	Dipropionato de betametasona	1801045-015787	1
Euro OTC	Dipropionato de betametasona	102001-012	1
Euro OTC	Dipropionato de betametasona	111007-01	1
Euro OTC	Dipropionato de betametasona	121002001	1
Euro OTC	Dipropionato de betametasona	1303006/01	1
Euro OTC	Dipropionato de betametasona	1303006-01	2
Euro OTC	Dipropionato de betametasona	1303006-02	1
Euro OTC	Dipropionato de betametasona	1305041-01	10
Euro OTC	Dipropionato de betametasona	1305041-02	3
Euro OTC	Dipropionato de betametasona	130541-01	1
Euro OTC	Dipropionato de betametasona	131023-02	1
Euro OTC	Dipropionato de betametasona	131102301	2
Euro OTC	Dipropionato de betametasona	1311023-01	11
Euro OTC	Dipropionato de betametasona	1311023-02	5
Euro OTC	Dipropionato de betametasona	13125702	1
Euro OTC	Dipropionato de betametasona	13372501	1
Euro OTC	Dipropionato de betametasona	1503003-01	10
Euro OTC	Dipropionato de betametasona	150300302	1
Euro OTC	Dipropionato de betametasona	1503003-02	12
Euro OTC	Dipropionato de betametasona	1506016-02	1
Euro OTC	Dipropionato de betametasona	15163304	1
Euro OTC	Dipropionato de betametasona	153003-01	1
Euro OTC	Dipropionato de betametasona	160103401	1
Euro OTC	Dipropionato de betametasona	1601034-01	25
Euro OTC	Dipropionato de betametasona	1610014-01	37
Euro OTC	Dipropionato de betametasona	1610014-015308	1
Euro OTC	Dipropionato de betametasona	17050-01	1
Euro OTC	Dipropionato de betametasona	170502001	1
Euro OTC	Dipropionato de betametasona	1705020-01	25
Euro OTC	Dipropionato de betametasona	17B16-B04-332218	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Dipropionato de betametasona	180104501	3
Euro OTC	Dipropionato de betametasona	1801045-01	27
Euro OTC	Dipropionato de betametasona	180808185	1
Euro OTC	Dipropionato de betametasona	1811007	1
Euro OTC	Dipropionato de betametasona	181100701	2
Euro OTC	Dipropionato de betametasona	1811007-01	25
Euro OTC	Dipropionato de betametasona	19070324-01	1
Euro OTC	Dipropionato de betametasona	1907034	1
Euro OTC	Dipropionato de betametasona	190703401	1
Euro OTC	Dipropionato de betametasona	1907034-01	32
Euro OTC	Dipropionato de betametasona	1907234-01	1
Euro OTC	Dipropionato de betametasona	20030057-01	1
Euro OTC	Dipropionato de betametasona	2003024-01	1
Euro OTC	Dipropionato de betametasona	200305-01	1
Euro OTC	Dipropionato de betametasona	2003057	1
Euro OTC	Dipropionato de betametasona	2003057-01	31
Euro OTC	Dipropionato de betametasona	2102001-01	21
Euro OTC	Dipropionato de betametasona	211000-01	1
Euro OTC	Dipropionato de betametasona	2110005-01	15
Euro OTC	Dipropionato de betametasona	2110005-02	5
Euro OTC	Dipropionato de betametasona	2208030-01	12
Euro OTC	Dipropionato de betametasona	2208030-1	1
Euro OTC	Dipropionato de betametasona	2208630-01	1
Euro OTC	Dipropionato de betametasona	BDP102/0817	1
Euro OTC	Dipropionato de betametasona	C0044/1A170130	1
euro//Noweda	Dipropionato de betametasona	1705030-01	1
EUro/AHD	Dipropionato de betametasona	1303006-01	3
Euro/Gehe	Dipropionato de betametasona	1601034-01	1
Euro/Gehe	Dipropionato de betametasona	2102001	1
Euro/Krieger	Dipropionato de betametasona	1801045-01	1
Euro/Phönix	Dipropionato de betametasona	2208030-01	1
Euro/Sanacorp	Dipropionato de betametasona	1503003-02	1
Fagon/Noweda	Dipropionato de betametasona	18I27-B03	1
Fagron	Dipropionato de betametasona		7
Fagron	Dipropionato de betametasona	10E19-N03	1
Fagron	Dipropionato de betametasona	11D26-N06	2
Fagron	Dipropionato de betametasona	11I02-N01	1
Fagron	Dipropionato de betametasona	11K28-N10	2
Fagron	Dipropionato de betametasona	12827-N08	1
Fagron	Dipropionato de betametasona	12B27-N08	6
Fagron	Dipropionato de betametasona	12C21-N13	1
Fagron	Dipropionato de betametasona	13/17-n05	1
Fagron	Dipropionato de betametasona	13/17-N05	15
Fagron	Dipropionato de betametasona	13023004	1
Fagron	Dipropionato de betametasona	1317-N05	1
Fagron	Dipropionato de betametasona	13i17-N05	1
Fagron	Dipropionato de betametasona	13I17-N05	12
Fagron	Dipropionato de betametasona	13j16-B01-291844	1
Fagron	Dipropionato de betametasona	13j16-b01-291845	1
Fagron	Dipropionato de betametasona	13J16-B01-291845	2
Fagron	Dipropionato de betametasona	14C03-B03-296838	1
Fagron	Dipropionato de betametasona	14C03-B06	2
Fagron	Dipropionato de betametasona	14C03-B06-296837	10
Fagron	Dipropionato de betametasona	15H25-B06-313088	1
Fagron	Dipropionato de betametasona	15H28B06313088	1
Fagron	Dipropionato de betametasona	15H28-B06-313088	4
Fagron	Dipropionato de betametasona	1601034-01	1
Fagron	Dipropionato de betametasona	16C04-B03	1
Fagron	Dipropionato de betametasona	16C04-B03-320850	5
Fagron	Dipropionato de betametasona	16C04-B03-320851	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dipropionato de betametasona	16C04-B03-320852	1
Fagron	Dipropionato de betametasona	17816B04332224	1
Fagron	Dipropionato de betametasona	17B16-B04	1
Fagron	Dipropionato de betametasona	17B16-B04-332217	9
Fagron	Dipropionato de betametasona	17b16b04332218	1
Fagron	Dipropionato de betametasona	17B16-B04-332219-201	1
Fagron	Dipropionato de betametasona	17B16-B04-332224	4
Fagron	Dipropionato de betametasona	17B6-B04-332217	1
Fagron	Dipropionato de betametasona	17E22-B06-335244	3
Fagron	Dipropionato de betametasona	17E22-B06-336705	2
Fagron	Dipropionato de betametasona	17E22B06336993	1
Fagron	Dipropionato de betametasona	17E22-B06-336993	5
Fagron	Dipropionato de betametasona	17H16-B04-340537	1
Fagron	Dipropionato de betametasona	18/27-B03-357221	2
Fagron	Dipropionato de betametasona	1801045-01	1
Fagron	Dipropionato de betametasona	1811007-01	1
Fagron	Dipropionato de betametasona	18127-B03-362601	1
Fagron	Dipropionato de betametasona	18127-B03-362603	1
Fagron	Dipropionato de betametasona	1827-b03-362601	1
Fagron	Dipropionato de betametasona	18B06-B05	5
Fagron	Dipropionato de betametasona	18B06-B05_350473	1
Fagron	Dipropionato de betametasona	18B06-B05-346218	5
Fagron	Dipropionato de betametasona	18B06-B05-346219	1
Fagron	Dipropionato de betametasona	18B06B05347338	1
Fagron	Dipropionato de betametasona	18B06-B05-347338	5
Fagron	Dipropionato de betametasona	18B06B0534996	1
Fagron	Dipropionato de betametasona	18b06-b05-350473	1
Fagron	Dipropionato de betametasona	18B06-B05-350473	10
Fagron	Dipropionato de betametasona	18B06-B05-350474	1
Fagron	Dipropionato de betametasona	18B06B05352731	2
Fagron	Dipropionato de betametasona	18B06-B05-352731	5
Fagron	Dipropionato de betametasona	18B06B05354807	1
Fagron	Dipropionato de betametasona	18B06-B05-354807	6
Fagron	Dipropionato de betametasona	18B06-B05-354808	3
Fagron	Dipropionato de betametasona	18Bo6-B0o5-352731	1
Fagron	Dipropionato de betametasona	18I127-B03-357222	1
Fagron	Dipropionato de betametasona	18I27-B03	8
Fagron	Dipropionato de betametasona	18I27-B03-357221	4
Fagron	Dipropionato de betametasona	18I27-B03-357222	3
Fagron	Dipropionato de betametasona	18I27-B03-358725	3
Fagron	Dipropionato de betametasona	18I27-B03-358726	1
Fagron	Dipropionato de betametasona	18I27-B03-358727	1
Fagron	Dipropionato de betametasona	18I27-B03-3626001	1
Fagron	Dipropionato de betametasona	18I27-B03-362601	10
Fagron	Dipropionato de betametasona	18I27-B03-362602	2
Fagron	Dipropionato de betametasona	18I27-B03-362602	1
Fagron	Dipropionato de betametasona	18127-B03-358725	1
Fagron	Dipropionato de betametasona	19041706	1
Fagron	Dipropionato de betametasona	19J31-F02	3
Fagron	Dipropionato de betametasona	19J31-F02-3666808	1
Fagron	Dipropionato de betametasona	19J31F02-366807	1
Fagron	Dipropionato de betametasona	19J31-F02-366807	7
Fagron	Dipropionato de betametasona	19J31-F02-366808	9
Fagron	Dipropionato de betametasona	19J31-F02-366809	1
Fagron	Dipropionato de betametasona	19J31-F02-366810	2
Fagron	Dipropionato de betametasona	20171127Ma5	1
Fagron	Dipropionato de betametasona	20C10_F02372115	1
Fagron	Dipropionato de betametasona	20C10-F02	1
Fagron	Dipropionato de betametasona	20C10-F02372115	1
Fagron	Dipropionato de betametasona	20C10-F02-372115	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dipropionato de betametasona	2109DM0B0011322	1
Fagron	Dipropionato de betametasona	21C002-F01-377438	1
Fagron	Dipropionato de betametasona	21C02-F01-3774308	1
Fagron	Dipropionato de betametasona	21C02-F01-377438	1
Fagron	Dipropionato de betametasona	21H18-B04-213656	8
Fagron	Dipropionato de betametasona	21J12-B09-216139	6
Fagron	Dipropionato de betametasona	21K24B04216140	2
Fagron	Dipropionato de betametasona	21K24-B04-216140	1
Fagron	Dipropionato de betametasona	21K24-B04-220120	2
Fagron	Dipropionato de betametasona	21K24-B04-222402	1
Fagron	Dipropionato de betametasona	21K24-B04-227289	2
Fagron	Dipropionato de betametasona	8K03-N13	1
Fagron	Dipropionato de betametasona	9J05-N09	1
Fagron	Dipropionato de betametasona	B03-3587205	1
Fagron	Dipropionato de betametasona	BDP003/0521	2
Fagron	Dipropionato de betametasona	BDP004/0821	1
Fagron	Dipropionato de betametasona	BDP101/0417	1
Fagron	Dipropionato de betametasona	BDP101/0419	2
Fagron	Dipropionato de betametasona	BDP102/0817	3
Fagron	Dipropionato de betametasona	F01-3774308	1
Fagron	Dipropionato de betametasona	F02-0668007	1
Fagron	Dipropionato de betametasona	F02-3668007	1
Fagron	Dipropionato de betametasona	F02-3721105	1
Fargon/ Noweda	Dipropionato de betametasona	13/17-N05	1
Fargon/AllianceH.	Dipropionato de betametasona	17H16B04-340537	1
Fargon	Dipropionato de betametasona	16C04-B033-24513	1
Fargon	Dipropionato de betametasona	17b16-b04-332224	1
Fragon/ Gehe	Dipropionato de betametasona	18B06-B05	1
Fragon	Dipropionato de betametasona	18B06-B05-352731	1
Gehe amax	Dipropionato de betametasona	1610014-01	1
Gehe amax	Dipropionato de betametasona	17B16-B04-332217	1
Gehe	Dipropionato de betametasona	1311023-01	1
Gehe	Dipropionato de betametasona	15238701	1
GEHE	Dipropionato de betametasona	15412914	1
Gehe	Dipropionato de betametasona	1705020-01	1
Gehe	Dipropionato de betametasona	17E22B06-336993	1
Gehe	Dipropionato de betametasona	18293404	1
GEHE	Dipropionato de betametasona	20003997005	1
Gehe	Dipropionato de betametasona	21000648001	1
Gehe	Dipropionato de betametasona	21000648010	1
Gehe	Dipropionato de betametasona	21000648012	1
Gehe	Dipropionato de betametasona	21k24-B04	1
Hirsch	Dipropionato de betametasona	1303006-01	1
Kehr	Dipropionato de betametasona	1705020-01	1
Kehr	Dipropionato de betametasona	220039602001	1
Klosterring	Dipropionato de betametasona	17B16-B04-332219	2
Nachprüfung	Dipropionato de betametasona	17B16-B04-332217	1
Noweda/ Caesar&Loren...	Dipropionato de betametasona	19000537003	1
Noweda	Dipropionato de betametasona	13236802	1
Noweda	Dipropionato de betametasona	13236803	1
Noweda	Dipropionato de betametasona	1811007-01	1
Noweda	Dipropionato de betametasona	21C02-F01-377438	1
Noweda	Dipropionato de betametasona	22001649008	1
Noweda	Dipropionato de betametasona	23011013-01	1
Noweda	Dipropionato de betametasona	BDP014/1115	1
Noweda	Dipropionato de betametasona	BDP102/0817	1
Ph/Euro	Dipropionato de betametasona	2110005-01	1
Phoenix 03.04.20147	Dipropionato de betametasona	13236805	1
Phoenix	Dipropionato de betametasona	13236806	1
Phoenix	Dipropionato de betametasona	1610014-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Dipropionato de betametasona	1705020-01	1
Phoenix	Dipropionato de betametasona	1811007-01	1
Phoenix	Dipropionato de betametasona	21000648006	1
Phönix Gotha	Dipropionato de betametasona	1811007-01	1
phönix	Dipropionato de betametasona	15163304	1
Phönix	Dipropionato de betametasona	1705020-01	1
PHÖNIX	Dipropionato de betametasona	17353603	1
Phönix	Dipropionato de betametasona	2003057-01	1
phönix	Dipropionato de betametasona	21000648014	1
Phönix	Dipropionato de betametasona	22001649005	1
sanacorb	Dipropionato de betametasona	12B27-No8	1
Sanacorp WE: 12.08.1…	Dipropionato de betametasona	15238701	1
Sanacorp	Dipropionato de betametasona	15412910	1
Sanacorp	Dipropionato de betametasona	1610014-01	1
Sanacorp	Dipropionato de betametasona	170502001	1
Sanacorp	Dipropionato de betametasona	1705020-01	1
Sanacorp	Dipropionato de betametasona	17105911	1
Sanacorp	Dipropionato de betametasona	17B16-B04-332217	2
Sanacorp	Dipropionato de betametasona	18090607	1
SANACORP	Dipropionato de betametasona	18293404	1
Sanacorp	Dipropionato de betametasona	18B06-B05-346218	1
Sanacorp	Dipropionato de betametasona	19000537010	1
Sanacorp	Dipropionato de betametasona	21000648010	1
Sanacorp	Dipropionato de betametasona	BDP102/0817	1
Symbiotica/Noweda	Dipropionato de betametasona	BDP102/0817	1
Symbiotica	Dipropionato de betametasona	2003057-01	2
Symbiotica	Dipropionato de betametasona	2208030-01	1
Symbiotica	Dipropionato de betametasona	BDP103/1019	1
WE:05.04.2016 Phönix	Dipropionato de betametasona	15163304	4
WE:09.12.2016	Dipropionato de betametasona	15163301	1

- 234 443 spectra from 1515 *Apo-Ident* customers from a total of 48 962 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dipropionato de betametasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dipropionato de betametasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	534	0	152 428
Type B	0	1293	0	200 791
Type C	0	1551	73	234 443

The substance/substance group *Dipropionato de betametasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8764 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5360 %)
Type C	100.0000 % (> 99.9007 %)	95.5049 % (> 95.3202 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20930	20930	0,00	39,63
20952	22372	8,46	38,31
21250	21250	0,00	38,12
21366	21250	5,41	38,46
21367	21250	5,99	39,15
21716	21716	0,00	38,96
22372	22372	0,00	37,10
22898	22372	7,89	39,40
25691	25691	0,00	42,14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ditranol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20032-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ditranol; Antralina; Dithranolum

Special notes

When selecting the *Ditranol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ditranol	11	5	155

Second-stage model

For differentiation of the substance/substance group *Ditranol* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ditranol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	114,21	–
⋮	⋮	⋮
Salicilato de sódio	>50	34,64
Cloreto de dequalínio	>50	36,10
Ácido acetilsalicílico	>50	51,98
Ácido benzoico	>50	59,17
Eosina amarela	>50	161,16
Cloridrato de oxitetraciclina	>50	269,52
Levotiroxina sódica	>50	567,21
Tanino	>50	1207,10

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ditranol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ditranol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ditranol	18115302	24169	40	1811302
Caelo	Ditranol	18190604	24429	40	1904372
Caelo	Ditranol	190868	24501	40	20190426*
Caelo	Ditranol	190550	24503	40	20190426*
Caelo	Ditranol	20002967002	25429	30	2102141
Caelo	Ditranol	20002967	25646	40	20201021*
Euro OTC	Ditranol	1702022-01	24153	40	1809448
Euro OTC	Ditranol	2201006	25960	40	20220209*
Fagron	Ditranol	18B23-B05-348137	24172	40	20180430
Fagron	Ditranol	20K20-B04-203566	25502	40	20201127
Fagron	Ditranol	22F11-B02-223754	26452	40	230502386

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 430 spectra of 11 reference samples from the substance/substance group *Ditranol*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 532 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 8 reference samples from the substance/substance group *Ditranol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Ditranol	APOP_DNL/11/17/001D	24173	40
Caelo	Ditranol	24000565	27320	40
Euro OTC	Ditranol	2001025	25101	40
Euro OTC	Ditranol	2004028	25472	40
Euro OTC	Ditranol	2409010	27455	40
Caelo	Ditranol	24000565	27320SI	20
Euro OTC	Ditranol	2201006	25960SI†	10
Euro OTC	Ditranol	2409010	27455SI	20

- 201 834 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 566 spectra from 385 *Apo-Ident* customers from 169 batches from the substance/substance group *Ditranol*.
- Among them are spectra of independent samples from 154 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ditranol	21000824004301221/4	1
	Ditranol	21I17-B01-213565	1
	Ditranol	22001422005	11
	Ditranol	22001422012	1
	Ditranol	2200142205	1
	Ditranol	2201006-01	1
	Ditranol	2201006-04	5
	Ditranol	2201006-05	2
	Ditranol	22F11-B02-219586	1
	Ditranol	22F11-B02-226170	5
	Ditranol	23F15-B01-231257	1
	Ditranol	23F15-BO1-231257	1
	Ditranol	23H22-B11-237978	1
	Ditranol	24000565004	2
	Ditranol	24F28-B29-002279	1
	Ditranol	B29-0022708	1
	Ditranol	OP-DNL-C1-001/22	1
11,41	Ditranol	23F15-B01-231257	1
AHC	Ditranol	2201006-01	1
AHD	Ditranol	1702022-04	1
AHD	Ditranol	21000824001	1
AHD	Ditranol	22001422005	1
AHD	Ditranol	APDT/386/2012D	1
Alliance	Ditranol	22001006-05	1
Alliance	Ditranol	22001422005	1
Alliance	Ditranol	2201006-05	1
Anzag	Ditranol		2
Anzag	Ditranol	120302502	1
Audor Pharma	Ditranol		15
Audor Pharma	Ditranol	11/11/002D	1
Audor Pharma	Ditranol	28(APOP-DNL/11/17/0	1
Audor Pharma	Ditranol	AOOP-DNL/11/17002S	1
Audor Pharma	Ditranol	APDT/351/2010D	1
Audor Pharma	Ditranol	APDT/365/2011	2
Audor Pharma	Ditranol	APDT/365/2011D	1
Audor Pharma	Ditranol	APDT/375/2012D	8
Audor Pharma	Ditranol	APDT/450/2016D	1
Audor Pharma	Ditranol	APDT/471/2017D	5
Audor Pharma	Ditranol	APDT3752012D	1
Audor Pharma	Ditranol	APDT3902013D	1
Audor Pharma	Ditranol	APO-DNL/11/17/001-1D	1
Audor Pharma	Ditranol	APOP-DNL/11/17/0002	1
Audor Pharma	Ditranol	ApOPDNL/11/17/001	1
Audor Pharma	Ditranol	APOP-DNL/11/17/001	2
Audor Pharma	Ditranol	APOP-DNL/11/17/001-1	3
Audor Pharma	Ditranol	APOPDNL/11/17/001-1D	1
Audor Pharma	Ditranol	APOP-DNL/11/17/001D	4

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Ditranol	APOP-DNL/11/17/001-D	4
Audor Pharma	Ditranol	APOP-DNL/11/17/002	4
Audor Pharma	Ditranol	apop-dnl/11/17/002d	1
Audor Pharma	Ditranol	APOP-DNL/11/17/002D	2
Audor Pharma	Ditranol	APOP-DNL/11/17001-1	1
Audor Pharma	Ditranol	APOP-DNL/11/17001-1D	1
Audor Pharma	Ditranol	APOP-DNL11170011D	1
Audor Pharma	Ditranol	APOPDNL1117002D	1
Audor Pharma	Ditranol	APQP-DNL/11/17/002D	1
Audor Pharma	Ditranol	DT/351/2010D	1
Audor Pharma	Ditranol	DT/375/2012D	2
Audor Pharma	Ditranol	OP-DNL/11/17/0001	1
Audor Pharma	Ditranol	OP-DNL/11/17/001	1
Audor Pharma	Ditranol	OP-DNL/11/17/001-1D	1
Caelo	Ditranol		2
Caelo	Ditranol	11064501	1
Caelo	Ditranol	12014502	1
Caelo	Ditranol	12014504	2
Caelo	Ditranol	1203025-02	1
Caelo	Ditranol	1212I-01274	1
Caelo	Ditranol	12236809	1
Caelo	Ditranol	12236811	4
Caelo	Ditranol	12375302	4
Caelo	Ditranol	12375305	1
Caelo	Ditranol	12375403	1
Caelo	Ditranol	12375601	1
Caelo	Ditranol	13120502	1
Caelo	Ditranol	13120503	1
Caelo	Ditranol	13120504	1
Caelo	Ditranol	13120702	1
Caelo	Ditranol	14101715	1
Caelo	Ditranol	1702022-01	1
Caelo	Ditranol	1702022-04	1
Caelo	Ditranol	18055001	1
Caelo	Ditranol	18115302	3
Caelo	Ditranol	18115306	3
Caelo	Ditranol	18115308	3
Caelo	Ditranol	18B23-B05-348137	1
Caelo	Ditranol	19055001	7
Caelo	Ditranol	19086804	3
Caelo	Ditranol	19204604	3
Caelo	Ditranol	19204605	5
Caelo	Ditranol	192939004	11
Caelo	Ditranol	192939005	3
Caelo	Ditranol	200000243003	1
Caelo	Ditranol	20000243003	13
Caelo	Ditranol	200004097004	1
Caelo	Ditranol	20001097004	1
Caelo	Ditranol	20002967002	1
Caelo	Ditranol	20004097001	6
Caelo	Ditranol	20004097002	1
Caelo	Ditranol	20004097004	8
Caelo	Ditranol	210000824001	1
Caelo	Ditranol	210008240007	1
Caelo	Ditranol	21000824001	20
Caelo	Ditranol	21000824002	2
Caelo	Ditranol	21000824004	25
Caelo	Ditranol	21000824007	14
Caelo	Ditranol	2100824004	1
Caelo	Ditranol	27111206	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ditranol	7/2020	1
Caelo	Ditranol	APDT/3652011D	1
Caelo	Ditranol	APDT/375/2012D	3
Caelo	Ditranol	APOP-DNL/11/17/001-1	1
Caelo	Ditranol	B04-2035606	1
Caesar & Loretz GmbH...	Ditranol	192939004	1
Caesar & Loretz GmbH...	Ditranol	21000824004	1
Caesar & Loretz GmbH...	Ditranol	192939004	1
Caesar & Loretz GmbH...	Ditranol	20000243002	1
Caesar & Loretz GmbH...	Ditranol	21000824004	1
Caesar & Loretz GmbH/Gehe	Ditranol	21000824001	1
Caesar & Loretz GmbH/Gehe	Ditranol	21000824004	1
Caesar & Loretz GmbH/Gehe	Ditranol	21000824007	1
Caesar & Loretz GmbH...	Ditranol	21000824007	2
Caesar & Loretz GmbH...	Ditranol	20004097001	1
Caesar & Loretz GmbH...	Ditranol	21000824002	1
Caesar & Loretz GmbH...	Ditranol	20000243004	1
Caesar & Loretz GmbH...	Ditranol	20004097001	1
Caesar & Loretz GmbH...	Ditranol	21000824007	2
Caesar & Loretz GmbH	Ditranol	1702022-04	1
Caesar & Loretz GmbH	Ditranol	19055001	2
Caesar & Loretz GmbH	Ditranol	19086804	1
CAESAR & LORETZ GMBH	Ditranol	192939004	1
Caesar & Loretz GmbH	Ditranol	192939005	1
Caesar & Loretz GmbH	Ditranol	20000243003	3
Caesar & Loretz GmbH	Ditranol	20000243004	1
Caesar & Loretz GmbH	Ditranol	20002967002	1
Caesar & Loretz GmbH	Ditranol	20004097001	7
Caesar & Loretz GmbH	Ditranol	20004097002	2
Caesar & Loretz GmbH	Ditranol	20004097004	5
Caesar & Loretz GmbH	Ditranol	21000824001	5
Caesar & Loretz GmbH	Ditranol	21000824003	1
Caesar & Loretz GmbH	Ditranol	21000824004	5
Caesar & Loretz GmbH	Ditranol	21000824007	3
Caesar & Loretz GmbH	Ditranol	22001422002	1
Caesar & Loretz GmbH	Ditranol	22001422005	1
Cealo	Ditranol	20004097004	2
Ceasar & Loretz GmbH...	Ditranol	19204605	1
EuRho / Noweda	Ditranol	2004028-01	1
EuRho/ Sanacorp	Ditranol	2201006-01	1
EuRho/Phoenix	Ditranol	2001025-01	2
EuRho/Sanacorp	Ditranol	2004028	1
EuRho	Ditranol	1203025-01	1
EuRho	Ditranol	2201006-03	1
Euro OTC	Ditranol		1
Euro OTC	Ditranol	1008011-01	1
Euro OTC	Ditranol	1008011-02	2
Euro OTC	Ditranol	1203025-01	2
Euro OTC	Ditranol	1203025-02	14
Euro OTC	Ditranol	1311029-01	1
Euro OTC	Ditranol	1702002-04	1
Euro OTC	Ditranol	17020022-02	1
Euro OTC	Ditranol	170202-01	1
Euro OTC	Ditranol	1702021	1
Euro OTC	Ditranol	1702021-02	2
Euro OTC	Ditranol	170202103	1
Euro OTC	Ditranol	1702021-03	13
Euro OTC	Ditranol	1702021-0301/2021	1
Euro OTC	Ditranol	1702022-01	2
Euro OTC	Ditranol	1702022-02	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Ditranol	1702022-04	12
Euro OTC	Ditranol	20004097002	1
Euro OTC	Ditranol	200102501	2
Euro OTC	Ditranol	2001025-01	26
Euro OTC	Ditranol	200402801	1
Euro OTC	Ditranol	2004028-01	6
Euro OTC	Ditranol	2004028-02	9
Euro OTC	Ditranol	2201006-01	5
Euro OTC	Ditranol	2201006-02	1
Euro OTC	Ditranol	2201006-03	7
Euro OTC	Ditranol	2201006-05	1
Euro OTC	Ditranol	56/11072013	1
Euro OTC	Ditranol	DT/370/2012	1
Euro OTC	Ditranol	DTHX-094	1
Euro/ AHC	Ditranol	2201006-03	1
Euro/ Gehe	Ditranol	APOP-DNL/11/17/002	1
Euro/Jenne	Ditranol	1702022-04	1
Fagron	Ditranol	11L20-N13	1
Fagron	Ditranol	1-21883004	1
Fagron	Ditranol	1218834	1
Fagron	Ditranol	13A30-N01	4
Fagron	Ditranol	17710I-01274	1
Fagron	Ditranol	18823-B50-35511	1
Fagron	Ditranol	18B23-B50-355511	2
Fagron	Ditranol	20C20-B07-200565	1
Fagron	Ditranol	20G27-B01-200443	2
Fagron	Ditranol	20K20-B04	1
Fagron	Ditranol	20K20-B04-203566	1
Fagron	Ditranol	20k20-B04-210534	1
Fagron	Ditranol	20K20-B04-210534	1
Fagron	Ditranol	21/17-B01-213565	1
Fagron	Ditranol	21/17-B01-218834	6
Fagron	Ditranol	21117-801-218834	1
Fagron	Ditranol	21117B01-218834	1
Fagron	Ditranol	21I17-b01-218834	1
Fagron	Ditranol	21I17-B01-218834	4
Fagron	Ditranol	220100603	1
Fagron	Ditranol	22F11-B02-226170	2
Fagron	Ditranol	22F11-BO2-226170	1
Fagron	Ditranol	9K10-N19	1
Fagron	Ditranol	B01-2188304	2
Fagron	Ditranol	BO1-2188304	1
Fagron	Ditranol	OP-DNL-C1-002/21	1
Gehe/Audar	Ditranol	APDT3752012D	1
Gehe/Euro	Ditranol	2201006-03	1
Gehe	Ditranol	1311029-01	1
Gehe	Ditranol	21/17-B01-218834	1
Gehe	Ditranol	22F11-B02-226170	2
Gehe	Ditranol	23F15-B01-231257	1
Gehe	Ditranol	APOP-DNL/11/17/001	1
Jenne / Optimus	Ditranol	2004028-01	1
Jenne	Ditranol	2001025-01	2
jenne	Ditranol	2201006-5	1
Kehr	Ditranol	22F11-B02-226170	1
Kehr	Ditranol	23F15-B01-235539	1
Noweda, EuRho	Ditranol	2201006-03	1
Noweda	Ditranol	1203025-02	1
Noweda	Ditranol	1702022-02	1
Noweda	Ditranol	2201006-04	1
Noweda	Ditranol	22F11-B02-219586	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Ditranol	APDT/375/2012	1
Noweda	Ditranol	DT/375/2012D	1
Optimus Pharma	Ditranol		1
Optimus/Phönix	Ditranol	APOP-DNL11/17/002D	1
Pala	Ditranol	DTHX-097	1
Phoenix/Noweda	Ditranol	APOP-DNL/11/17/002D	1
Phoenix	Ditranol	1701030-01	1
Phoenix	Ditranol	apopdnl11117002d	1
phönix	Ditranol	21000824007	1
Phönix	Ditranol	2201006-05	1
Phönix	Ditranol	Caelo	1
Sanacorp	Ditranol		1
Sanacorp	Ditranol	1702022-04	1
Sanacorp	Ditranol	20K20-B04-210534	1
Sanacorp	Ditranol	21I17B01-213565	1
Sanacorp	Ditranol	22001422005	2
Sanacorp	Ditranol	APDT/375/2012	1
Sanacorp	Ditranol	APOP-DNL/11/17/001-D	1

- 235 501 spectra from 1515 *Apo-Ident* customers from a total of 49 090 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ditranol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ditranol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	430	0	152 532
Type B	0	250	0	201 834
Type C	0	525	41	235 501

The substance/substance group *Ditranol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6047 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	92.7562 % (> 92.2261 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24153	24153	0,00	154,98
24169	24169	0,00	148,86
24172	24169	5,47	148,30
24429	24429	0,00	170,57
24501	24501	0,00	146,48
24503	24503	0,00	149,02
25429	25429	0,00	164,43
25502	24153	30,41	144,98
25646	25646	0,00	173,47
25960	25960	0,00	209,55
26452	26452	0,00	151,70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**DL metionina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10004593-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

DL metionina; DL-Methioninum; Metionina (DL)

Special notes

When selecting the *DL metionina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
DL metionina	3	1	2

Second-stage model

For differentiation of the substance/substance group *DL metionina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *DL metionina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aspartato de ornitina	81,85	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *DL metionina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *DL metionina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	DL metionina	172575	25449	40	20171024*
Caelo	DL metionina	190211	25450	40	20190306*
Caelo	DL metionina	23000413	26714	40	20230323*
Caelo	DL metionina	23000413	26714SI	20	20230323*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *DL metionina*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 822 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *DL metionina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	DL metionina	193073	25451	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *DL metionina*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	DL metionina	16274007	1
Caelo	DL metionina	21000019005	2

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *DL metionina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *DL metionina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	40	0	202 044
Type C	0	3	0	236 064

The substance/substance group *DL metionina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25449	25449	0,00	121,24
25450	25450	0,00	117,38
26714	26714	0,00	128,29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Edetato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20937-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Edetato de sódio; Dinatrii edetas; EDTA dissódico

Special notes

When selecting the *Edetato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Edetato de sódio	7	17	236

Second-stage model

For differentiation of the substance/substance group *Edetato de sódio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Edetato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	97,73	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Edetato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Edetato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Edetato de sódio	13142009	21362	40	20130524
Caelo	Edetato de sódio	161364	22465	60	20160504*
Euro OTC	Edetato de sódio	1609023	22915	40	20170106*
Euro OTC	Edetato de sódio	1812016	24414	40	20190116*
Fagron	Edetato de sódio	13E15-N05	20937	40	1402193
Fagron	Edetato de sódio	16F21-B02-325085	22926	40	20160713
Fagron	Edetato de sódio	22G15-B01-224176	26394	40	20220803
Fagron	Edetato de sódio	22G15-B01-224176	26394SI	20	20220803

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Edetato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 20 reference samples from the substance/substance group *Edetato de sódio*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Edetato de sódio	172618	23663	40
Caelo	Edetato de sódio	20001878	25209	40
Caelo	Edetato de sódio	21001224	25803	40
Caelo	Edetato de sódio	22003154	26486	40
Caelo	Edetato de sódio	24001067	27329	40
Euro OTC	Edetato de sódio	1609023-01	22950	40
Euro OTC	Edetato de sódio	1704011	23390	40
Euro OTC	Edetato de sódio	1806007	24157	40
Euro OTC	Edetato de sódio	1807025	24159	40
Euro OTC	Edetato de sódio	1901032	24472	40
Euro OTC	Edetato de sódio	1909030	24958	40
Euro OTC	Edetato de sódio	2004003	25168	40
Euro OTC	Edetato de sódio	2008009	25314	40
Euro OTC	Edetato de sódio	2205014	26188	40
Euro OTC	Edetato de sódio	2209004	26335	40
Euro OTC	Edetato de sódio	2402026	27155	40
Fagron	Edetato de sódio	24C25-B37-001217	27380	40
Caelo	Edetato de sódio	172618	23818	40
Euro OTC	Edetato de sódio	2205014	26188SI	20
Euro OTC	Edetato de sódio	2209004	26335SI	20

- 201 324 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

provided by the customer regarding manufacturer and batch number.

- 1044 spectra from 591 *Apo-Ident* customers from 250 batches from the substance/substance group *Edetato de sódio*.
- Among them are spectra of independent samples from 236 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Edetato de sódio		1
	Edetato de sódio	13142009	1
	Edetato de sódio	20004094011	1
	Edetato de sódio	21001224017	1
	Edetato de sódio	21122-F04-380679	1
	Edetato de sódio	21H12-B03-213591	2
	Edetato de sódio	21H12-B03-215577	1
	Edetato de sódio	21I22-F04-380679	1
	Edetato de sódio	21L06-B01	1
	Edetato de sódio	21L06-B01-217364	5
	Edetato de sódio	22000319007	7
	Edetato de sódio	22000319008	1
	Edetato de sódio	22003154003	3
	Edetato de sódio	22003154005	1
	Edetato de sódio	23A27-B01-230833	1
	Edetato de sódio	23A27-B01-235141	1
	Edetato de sódio	23A27-B01-235142	1
	Edetato de sódio	24C25-B37-001217	1
Alliance Healthcare	Edetato de sódio	12181714	1
Alliance Healthcare	Edetato de sódio	13E15-N05	2
Alliance Healthcare	Edetato de sódio	21001224002	1
Anzag	Edetato de sódio	13K19-B02-290051	1
Anzag	Edetato de sódio	18H03-B04-358927	1
apoident	Edetato de sódio	1807044-01	1
apomix	Edetato de sódio	14G03-B05-307737	1
Bombastus	Edetato de sódio		1
Bombastus	Edetato de sódio	16136404	1
Caelo	Edetato de sódio		1
Caelo	Edetato de sódio	10887102	1
Caelo	Edetato de sódio	11074608	2
Caelo	Edetato de sódio	11074703	1
Caelo	Edetato de sódio	12181702	1
Caelo	Edetato de sódio	12181703	3
Caelo	Edetato de sódio	12181704	1
Caelo	Edetato de sódio	12181706	2
Caelo	Edetato de sódio	12181711	13
Caelo	Edetato de sódio	12181714	4
Caelo	Edetato de sódio	12254507	2
Caelo	Edetato de sódio	12345	1
Caelo	Edetato de sódio	12E16-N04	1
Caelo	Edetato de sódio	13/23-N03-3472312131	1
Caelo	Edetato de sódio	13142002	4
Caelo	Edetato de sódio	13142004	4
Caelo	Edetato de sódio	13142008	6
Caelo	Edetato de sódio	13142009	11
Caelo	Edetato de sódio	13142010	2
Caelo	Edetato de sódio	13142014	1
Caelo	Edetato de sódio	13142015	5
Caelo	Edetato de sódio	13142018	2
Caelo	Edetato de sódio	13395002	3
Caelo	Edetato de sódio	13395007	4
Caelo	Edetato de sódio	13E15-N05	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Edetato de sódio	13E15-N05	1
Caelo	Edetato de sódio	13K19-B02-290051	1
Caelo	Edetato de sódio	14031801	1
Caelo	Edetato de sódio	1427006	1
Caelo	Edetato de sódio	14270505	2
Caelo	Edetato de sódio	14270506	4
Caelo	Edetato de sódio	14G03-B05-307737	1
Caelo	Edetato de sódio	15035603	3
Caelo	Edetato de sódio	15035604	4
Caelo	Edetato de sódio	15116602	4
Caelo	Edetato de sódio	15116603	15
Caelo	Edetato de sódio	1517E-01925	1
Caelo	Edetato de sódio	15427703	15
Caelo	Edetato de sódio	15427704	5
Caelo	Edetato de sódio	15427705	4
Caelo	Edetato de sódio	15427710	13
Caelo	Edetato de sódio	15427712	1
Caelo	Edetato de sódio	15427714	25
Caelo	Edetato de sódio	15427717	11
Caelo	Edetato de sódio	1547717	1
Caelo	Edetato de sódio	16110103/1	1
Caelo	Edetato de sódio	16136403	4
Caelo	Edetato de sódio	16136404	5
Caelo	Edetato de sódio	16337302	9
Caelo	Edetato de sódio	16337305	3
Caelo	Edetato de sódio	16337312	24
Caelo	Edetato de sódio	16337313	2
Caelo	Edetato de sódio	16337316	14
Caelo	Edetato de sódio	166337312	1
Caelo	Edetato de sódio	16F21-B02-327696	1
Caelo	Edetato de sódio	17336102	22
Caelo	Edetato de sódio	17336107	5
Caelo	Edetato de sódio	17336115	25
Caelo	Edetato de sódio	17D25-B08	1
Caelo	Edetato de sódio	17d25-b08-339881	1
Caelo	Edetato de sódio	17D25-B08-341590	2
Caelo	Edetato de sódio	17D25-B08-343253	2
Caelo	Edetato de sódio	18007102	13
Caelo	Edetato de sódio	18007104	3
Caelo	Edetato de sódio	18007110	22
Caelo	Edetato de sódio	18007112	3
Caelo	Edetato de sódio	18007113	1
Caelo	Edetato de sódio	18H03-B03-353918	1
Caelo	Edetato de sódio	18H03-B04	1
Caelo	Edetato de sódio	18H03-B04-352162	3
Caelo	Edetato de sódio	18H03B04356574	1
Caelo	Edetato de sódio	18H03-B04-357771	3
Caelo	Edetato de sódio	191896007	21
Caelo	Edetato de sódio	19189603	7
Caelo	Edetato de sódio	200004094004	1
Caelo	Edetato de sódio	20004094001	10
Caelo	Edetato de sódio	20004094002	1
Caelo	Edetato de sódio	20004094004	17
Caelo	Edetato de sódio	20004094006	2
Caelo	Edetato de sódio	20004094011	4
Caelo	Edetato de sódio	20004424015	1
Caelo	Edetato de sódio	21001224002	1
Caelo	Edetato de sódio	21001224003	14
Caelo	Edetato de sódio	21001224005	8
Caelo	Edetato de sódio	21001224006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Edetato de sódio	21001224013	9
Caelo	Edetato de sódio	21001224015	9
Caelo	Edetato de sódio	21001224017	5
Caelo	Edetato de sódio	21001224019	1
Caelo	Edetato de sódio	21001224031	1
Caelo	Edetato de sódio	2100128002	1
Caelo	Edetato de sódio	2101414	1
Caelo	Edetato de sódio	22000319004	2
Caelo	Edetato de sódio	22000319007	4
Caelo	Edetato de sódio	220304NE	1
Caelo	Edetato de sódio	2913M1925	1
Caelo	Edetato de sódio	3211I-01925	1
Caelo	Edetato de sódio	3913A-01925	1
Caelo	Edetato de sódio	601EC350	1
Caelo	Edetato de sódio	601EF200	1
Caelo	Edetato de sódio	601EH014	1
Caelo	Edetato de sódio	92159379	1
Caelo	Edetato de sódio	B03-3617200	1
Caelo	Edetato de sódio	P-14011921/17336102	1
Caelo	Edetato de sódio	P-16061621/15427703	1
Caesar & Loretz GmbH...	Edetato de sódio	13142004	1
Caesar & Loretz GmbH...	Edetato de sódio	20004094004	1
Caesar & Loretz GmbH Og	Edetato de sódio	21001224017	1
Caesar & Loretz GmbH...	Edetato de sódio	12181711	1
Caesar & Loretz GmbH...	Edetato de sódio	20004094002	1
Caesar & Loretz GmbH...	Edetato de sódio	21001224005	1
Caesar & Loretz GmbH/GEHE	Edetato de sódio	17336115	1
Caesar & Loretz GmbH/Gehe	Edetato de sódio	21001224017	1
Caesar & Loretz GmbH...	Edetato de sódio	191896010	1
Caesar & Loretz GmbH...	Edetato de sódio	21000128002	1
Caesar & Loretz GmbH...	Edetato de sódio	21001224017	1
Caesar & Loretz GmbH/sana	Edetato de sódio	21000128002	1
Caesar & Loretz GmbH...	Edetato de sódio	16337316	1
Caesar & Loretz GmbH...	Edetato de sódio	18007112	1
Caesar & Loretz GmbH...	Edetato de sódio	191896007	1
Caesar & Loretz GmbH...	Edetato de sódio	21001224005	1
Caesar & Loretz GmbH	Edetato de sódio	13142008	1
Caesar & Loretz GmbH	Edetato de sódio	14270505	1
Caesar & Loretz GmbH	Edetato de sódio	15427705	1
Caesar & Loretz GmbH	Edetato de sódio	16337312	1
Caesar & Loretz GmbH	Edetato de sódio	17336115	6
Caesar & Loretz GmbH	Edetato de sódio	1736115	1
Caesar & Loretz GmbH	Edetato de sódio	18007102	1
Caesar & Loretz GmbH	Edetato de sódio	18007104	1
Caesar & Loretz GmbH	Edetato de sódio	18007110	4
Caesar & Loretz GmbH	Edetato de sódio	18007112	1
Caesar & Loretz GmbH	Edetato de sódio	18007113	4
Caesar & Loretz GmbH	Edetato de sódio	191896007	13
Caesar & Loretz GmbH	Edetato de sódio	19189603	3
Caesar & Loretz GmbH	Edetato de sódio	20004094001	4
Caesar & Loretz GmbH	Edetato de sódio	20004094004	13
Caesar & Loretz GmbH	Edetato de sódio	20004094006	3
Caesar & Loretz GmbH	Edetato de sódio	20004094011	2
Caesar & Loretz GmbH	Edetato de sódio	21001224002	2
Caesar & Loretz GmbH	Edetato de sódio	21001224003	1
Caesar & Loretz GmbH	Edetato de sódio	21001224005	2
Caesar & Loretz GmbH	Edetato de sódio	21001224012	1
Caesar & Loretz GmbH	Edetato de sódio	21001224013	3
Caesar & Loretz GmbH	Edetato de sódio	21001224015	5
Caesar & Loretz GmbH	Edetato de sódio	21001224017	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Edetato de sódio	21001224019	1
Caesar & Loretz GmbH	Edetato de sódio	22000319004	1
Carl Roth	Edetato de sódio	159280302	1
Celo/Noweda	Edetato de sódio	18007102	1
Ceolo	Edetato de sódio	1909030-01	1
Cranach-Apotheke	Edetato de sódio	11a31-no6	1
Delta Apotheke	Edetato de sódio	18007102	2
Euro OTC	Edetato de sódio	13142018	2
Euro OTC	Edetato de sódio	15427703	1
Euro OTC	Edetato de sódio	16337312	1
Euro OTC	Edetato de sódio	190903001	1
Euro OTC	Edetato de sódio	1909030-01	2
Euro OTC	Edetato de sódio	2004003-01	1
Euro OTC	Edetato de sódio	21001224013	1
Euro OTC	Edetato de sódio	E300033328	1
Fagron	Edetato de sódio	11A31-N06	1
Fagron	Edetato de sódio	11A31-N06Retest	1
Fagron	Edetato de sódio	12E12-N04	1
Fagron	Edetato de sódio	12E16-N04	2
Fagron	Edetato de sódio	12g25-n12	1
Fagron	Edetato de sódio	12G25-N12	3
Fagron	Edetato de sódio	13/23-N03	6
Fagron	Edetato de sódio	13E15-B10-289034	1
Fagron	Edetato de sódio	13E15-N05	10
Fagron	Edetato de sódio	13G15-N03	4
Fagron	Edetato de sódio	13I23-N03	10
Fagron	Edetato de sódio	13I23-NO3	1
Fagron	Edetato de sódio	13K19B02	1
Fagron	Edetato de sódio	13K19-B02	1
Fagron	Edetato de sódio	13K19-B02-289035	1
Fagron	Edetato de sódio	13k19-b02-290051	2
Fagron	Edetato de sódio	13K19B02290051	1
Fagron	Edetato de sódio	13K19-B02-290051	11
Fagron	Edetato de sódio	13K19-B02-290052	3
Fagron	Edetato de sódio	13K19-B02-296324	1
Fagron	Edetato de sódio	14G03-B05	5
Fagron	Edetato de sódio	14G03-B05_307737	1
Fagron	Edetato de sódio	14G03-B05-303420	1
Fagron	Edetato de sódio	14G03-B05-303422	1
Fagron	Edetato de sódio	14G03-B05-30773	1
Fagron	Edetato de sódio	14G03-B05-307737	8
Fagron	Edetato de sódio	14G03B05309971	1
Fagron	Edetato de sódio	14G03-B05-309971	2
Fagron	Edetato de sódio	15D01-B05-315877	4
Fagron	Edetato de sódio	15D01-B05-317369	2
Fagron	Edetato de sódio	164599-0001	1
Fagron	Edetato de sódio	16F21-B02	3
Fagron	Edetato de sódio	16F21-B02-323069	1
Fagron	Edetato de sódio	16F21-B02-323074	2
Fagron	Edetato de sódio	16F21-B02-324370	4
Fagron	Edetato de sódio	16f21b02325085	1
Fagron	Edetato de sódio	16F21-B02-325085	6
Fagron	Edetato de sódio	16F21-B02-325891	3
Fagron	Edetato de sódio	16f21-b02-327696	1
Fagron	Edetato de sódio	16F21B02327696	1
Fagron	Edetato de sódio	16F21-B02-327696	5
Fagron	Edetato de sódio	16F21-B02-329900	5
Fagron	Edetato de sódio	16f21-b02-330959	1
Fagron	Edetato de sódio	16F21-B02-332039	1
Fagron	Edetato de sódio	16F21-B02-333607	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Edetato de sódio	16F21-B02-333610	3
Fagron	Edetato de sódio	17D25-B08	4
Fagron	Edetato de sódio	17D25-B08-334827	4
Fagron	Edetato de sódio	17D25-B08-334827	1
Fagron	Edetato de sódio	17D25-B08-336718	4
Fagron	Edetato de sódio	17D25-B08-338202	4
Fagron	Edetato de sódio	17D25-B08-339881	4
Fagron	Edetato de sódio	17D25B08343253	1
Fagron	Edetato de sódio	17D25-B08-343253	4
Fagron	Edetato de sódio	17D25-B08-343254	1
Fagron	Edetato de sódio	17D25-Bo8-336718	1
Fagron	Edetato de sódio	18H03	1
Fagron	Edetato de sódio	18H03-B04	3
Fagron	Edetato de sódio	18H03-B04-352162	1
Fagron	Edetato de sódio	18H03-B04-353034	8
Fagron	Edetato de sódio	18H03-B04-353918	6
Fagron	Edetato de sódio	18H03-B04-355280	7
Fagron	Edetato de sódio	18h03-b04-356574	1
Fagron	Edetato de sódio	18H03-B04-356574	6
Fagron	Edetato de sódio	18H03-B04-35674	1
Fagron	Edetato de sódio	18H03-B04-357771	8
Fagron	Edetato de sódio	18H03-B04-357774	8
Fagron	Edetato de sódio	18h03b04358927	1
Fagron	Edetato de sódio	18H03B04-358927	1
Fagron	Edetato de sódio	18H03-B04-358927	6
Fagron	Edetato de sódio	18H09-B04-355280	1
Fagron	Edetato de sódio	18K14-B03	5
Fagron	Edetato de sódio	18K14-B03-358930	13
Fagron	Edetato de sódio	18K14-B03-358931	1
Fagron	Edetato de sódio	18K14B03358934	1
Fagron	Edetato de sódio	18K14-B03-358934	4
Fagron	Edetato de sódio	18K14-B03-361720	16
Fagron	Edetato de sódio	18K14-B03-361721	1
Fagron	Edetato de sódio	20f23	1
Fagron	Edetato de sódio	20F23-F03	1
Fagron	Edetato de sódio	20F23-F03-372618	6
Fagron	Edetato de sódio	21/22-F04	1
Fagron	Edetato de sódio	21122-F04_380679	1
Fagron	Edetato de sódio	21122-F04-380105	1
Fagron	Edetato de sódio	2122-F04-380679	1
Fagron	Edetato de sódio	215I-01925	1
Fagron	Edetato de sódio	218U-01925	1
Fagron	Edetato de sódio	21I22-F04	2
Fagron	Edetato de sódio	21I22-F04_380679	1
Fagron	Edetato de sódio	21I22-F04-380105	1
Fagron	Edetato de sódio	21I22F04380679	1
Fagron	Edetato de sódio	21I22-F04-380679	10
Fagron	Edetato de sódio	21L06-B01-217364	1
Fagron	Edetato de sódio	352162	1
Fagron	Edetato de sódio	361720	1
Fagron	Edetato de sódio	-37261008	2
Fagron	Edetato de sódio	5012Q-01925	1
Fagron	Edetato de sódio	5218Q-01925	1
Fagron	Edetato de sódio	5315A-01925	1
Fagron	Edetato de sódio	601EB174	1
Fagron	Edetato de sódio	601EB262	1
Fagron	Edetato de sódio	601EC350	2
Fagron	Edetato de sódio	601EE047	3
Fagron	Edetato de sódio	601EF172	4
Fagron	Edetato de sódio	601EF200	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Edetato de sódio	601EHO14	1
Fagron	Edetato de sódio	601EI153	2
Fagron	Edetato de sódio	601H1300	2
Fagron	Edetato de sódio	601H9118	1
Fagron	Edetato de sódio	601HA062	6
Fagron	Edetato de sódio	6O1EI153	1
Fagron	Edetato de sódio	813Q-01925	1
Fagron	Edetato de sódio	914E-01925	1
Fagron	Edetato de sódio	B01-2173006	1
Fagron	Edetato de sódio	B03-2135901	1
Fagron	Edetato de sódio	B03-3617200	1
Fagron	Edetato de sódio	B03-3617201	1
Fagron	Edetato de sódio	F03-3726108	2
Fagron	Edetato de sódio	FO4-3806709	1
Fagron	Edetato de sódio	NE5736385	1
Fargo/Phönix	Edetato de sódio	18K14-BO3	1
Fargo/Sana	Edetato de sódio	20004094006	1
Fargon/Noweda	Edetato de sódio	18H03-B04-356574	2
Fargon/Phönix	Edetato de sódio	BO3-3617201	1
Fargon	Edetato de sódio	18H03-B04	1
Fargon	Edetato de sódio	18H03-B04-353034	1
Fargron / Noweda	Edetato de sódio	16f21-b0-330959	1
Fiebig	Edetato de sódio	16F21-B02-327696	1
Fiebig	Edetato de sódio	18007110	1
Fragon/Noweda	Edetato de sódio	18H03-B04-358927	1
Gehe	Edetato de sódio	13142018	1
Gehe	Edetato de sódio	13E15-N05	1
Gehe	Edetato de sódio	15427710	1
Gehe	Edetato de sódio	21L06-B01-217364	1
Gehe	Edetato de sódio	22003154005	1
Kehr/Fargon	Edetato de sódio	17d25-b08-343253	1
kehr	Edetato de sódio	17D25-B08-339881	1
Kehr	Edetato de sódio	21L06-B01	1
Noweda/Gehe	Edetato de sódio	14G03-B05-307737	1
Noweda	Edetato de sódio	15427710	1
Noweda	Edetato de sódio	16337312	1
Noweda	Edetato de sódio	18K14-B03-361720	1
Noweda	Edetato de sódio	601H1300	1
Noweda	Edetato de sódio	B03-3617200	1
Phoenix Goettin	Edetato de sódio	13G15-N03	1
Phoenix Goettin	Edetato de sódio	13G15-NO3	1
Phoenix	Edetato de sódio	15427704	1
Phoenix	Edetato de sódio	16F21-B02-333607	1
Phoenix	Edetato de sódio	18007110	1
Phoenix	Edetato de sódio	3411	1
Phönix	Edetato de sódio	11074702	1
Phönix	Edetato de sódio	13142004	1
phönix	Edetato de sódio	13142018	1
Phönix	Edetato de sódio	13E15-B10	1
Phönix	Edetato de sódio	13G15-N03	1
phönix	Edetato de sódio	13K19-B02-290051	1
phönix	Edetato de sódio	15427703	1
phönix	Edetato de sódio	15427704	1
Phönix	Edetato de sódio	164599-0001	1
Phönix	Edetato de sódio	16F21-B02-327696	1
Phönix	Edetato de sódio	18007110	1
Phönix	Edetato de sódio	18H03-B04-353034	1
Phönix	Edetato de sódio	18K14-B03-358930	2
Phönix	Edetato de sódio	200471805	1
Phönix	Edetato de sódio	601ef200	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Röntgen	Edetato de sódio	16337302	1
Röntgen	Edetato de sódio	20004094001	1
Sanacorp	Edetato de sódio	12G25-N12	2
Sanacorp	Edetato de sódio	13E15-N05	1
Sanacorp	Edetato de sódio	1505603	1
Sanacorp	Edetato de sódio	164599-0001	1
sanacorp	Edetato de sódio	16F21-B02-324370	1
Sanacorp	Edetato de sódio	17336115	1
Sanacorp	Edetato de sódio	20004094004	1
Sanacorp	Edetato de sódio	21h12-b03-213591	2
Sanacorp	Edetato de sódio	21i22-F04-380679	1
Sanacorp	Edetato de sódio	22000319007	1
Sanacorp	Edetato de sódio	6/AKD14	1
VDL	Edetato de sódio	22000319008	1
Vincenten/ Sanacorp	Edetato de sódio	18K14-B03-3617200	1

- 235 023 spectra from 1515 *Apo-Ident* customers from a total of 49 012 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Edetato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Edetato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	760	0	201 324
Type C	0	1042	2	235 023

The substance/substance group *Edetato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	99.8084 % (> 99.5211 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20937	20937	0,00	143,08
21362	22465	5,26	142,91
22465	22465	0,00	145,01
22915	22915	0,00	144,31
22926	22465	8,03	142,38
24414	24414	0,00	141,81
26394	20937	7,34	144,99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Edetato dissódico de cálcio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10003685-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Edetato dissódico de cálcio; EDTA dissódico de cálcio; Natrii calcii edetas

Special notes

When selecting the *Edetato dissódico de cálcio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Edetato dissódico de cálcio	6	2	3

Second-stage model

For differentiation of the substance/substance group *Edetato dissódico de cálcio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Edetato dissódico de cálcio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Monoestearato de glicerol, emulsionante	72,86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Edetato dissódico de cálcio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Edetato dissódico de cálcio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Edetato dissódico de cálcio	1807024	24145	40	20180725*
Euro OTC	Edetato dissódico de cálcio	1901028	24467	40	20190218*
Euro OTC	Edetato dissódico de cálcio	1910014	24955	40	20191119*
Euro OTC	Edetato dissódico de cálcio	2003032	25242	40	20200527*
Euro OTC	Edetato dissódico de cálcio	2207022	26266	40	20220818*
Euro OTC	Edetato dissódico de cálcio	2207022	26266SI	20	20220818*
Euro OTC	Edetato dissódico de cálcio	2301043	26593	40	20230309*
Euro OTC	Edetato dissódico de cálcio	2301043	26593SI	20	20230309*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 8 reference samples from the substance/substance group *Edetato dissódico de cálcio*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 3 reference samples from the substance/substance group *Edetato dissódico de cálcio*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Edetato dissódico de cálcio	1705029	23434	40
Euro OTC	Edetato dissódico de cálcio	2311016	27072	40
Euro OTC	Edetato dissódico de cálcio	2311016	27072SI	20

- 201 984 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 1 *Apo-Ident* customers from 4 batches from the substance/substance group *Edetato dissódico de cálcio*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Edetato dissódico de cálcio	1901028-01Retest	1
Euro OTC	Edetato dissódico de cálcio	1910014-01	1
Euro OTC	Edetato dissódico de cálcio	2003032	1
Euro OTC	Edetato dissódico de cálcio	2010022-01	3

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Edetato dissódico de cálcio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Edetato dissódico de cálcio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	100	0	201 984
Type C	0	6	0	236 061

The substance/substance group *Edetato dissódico de cálcio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24145	24145	0,00	182,93
24467	24467	0,00	131,75
24955	24955	0,00	210,47
25242	25242	0,00	176,74
26266	26266	0,00	201,77
26593	26593	0,00	207,26

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Eosina amarela**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20571-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Eosina amarela; Eosina amarelada; Eosina Y; Eosinum natricum

Special notes

When selecting the *Eosina amarela* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Eosina amarela	7	3	59

Second-stage model

For differentiation of the substance/substance group *Eosina amarela* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Eosina amarela* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	58,88	–
⋮	⋮	⋮
Cloreto de dequalínio	>50	58,19
Levotiroxina sódica	>50	62,34
Cloridrato de oxitetraciclina	>50	91,58
Tanino	>50	127,44
Salicilato de sódio	>50	276,47
Ditranol	>50	302,29
Ácido acetilsalicílico	>50	341,36
Ácido benzoico	>50	380,65

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Eosina amarela* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Eosina amarela*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Eosina amarela	12E25-N01	20900	60	20120607
Fagron	Eosina amarela	15G01-T03-025958	22261	60	1604114
Fagron	Eosina amarela	13F14-T01-017395	22534	40	1608469
Fagron	Eosina amarela	13F14-T01-017395	22535	40	20141219
Fagron	Eosina amarela	13F14-T01-017395	22660	40	1801115
Fagron	Eosina amarela	13F14-T01-017395	22816	40	1705197
Fagron	Eosina amarela	17K21-T07-042542	23975	40	1805338
Fagron	Eosina amarela	19J25-B06-196532	25187	40	20191216
Fagron	Eosina amarela	20G07-B02-200510	25503	40	20200730
Fagron	Eosina amarela	23E10-B02-228749	26822	40	20230619

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Eosina amarela*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Eosina amarela*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Eosina amarela	13I11-N03	20932	40
Fagron	Eosina amarela	20J13-B01-201856	25754	40
Fagron	Eosina amarela	21L20-B06-213987	26063	40
Fagron	Eosina amarela	13I11-N03	21208	40
Fagron	Eosina amarela	21L20-B06-213987	26063SI	20
Fagron	Eosina amarela	23E10-B02-228749	26822SI†	20

- 201 884 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 200 spectra from 170 *Apo-Ident* customers from 69 batches from the substance/substance group *Eosina amarela*.

- Among them are spectra of independent samples from 59 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Eosina amarela	21L20-B06	1
	Eosina amarela	21L20-B06-213987	1
	Eosina amarela	22I27-B01-223849	4
	Eosina amarela	22I27-B01-223850	1
	Eosina amarela	23E10-B02-228749	2
	Eosina amarela	B06-2139807	2
	Eosina amarela	EYWS/03/22	1
Cael Sanacorp 05.02.2016	Eosina amarela	13F14-T01-017395	1
Caelo	Eosina amarela	12e25n01	1
Caelo	Eosina amarela	12e25-n01	1
Caelo	Eosina amarela	13F14-T01-017395	1
Caelo	Eosina amarela	13I11-N03	1
Caelo	Eosina amarela	14H28-M05	1
Caelo	Eosina amarela	15G01-T03-025958	1
Caelo	Eosina amarela	17K21-T07	1
Caelo	Eosina amarela	20J13-B01-201856	1
Fagron	Eosina amarela	1(20G0-B02-200510)	1
Fagron	Eosina amarela	11E25-N01	1
Fagron	Eosina amarela	11F21-N10	1
Fagron	Eosina amarela	12A02-N09	2
Fagron	Eosina amarela	12E25-N01	4
Fagron	Eosina amarela	12H28-N08	3
Fagron	Eosina amarela	13/11-N03	3
Fagron	Eosina amarela	13/11-NO3	1
Fagron	Eosina amarela	13F14-T01-017395	6
Fagron	Eosina amarela	13fF14-T01-017395	1
Fagron	Eosina amarela	14H28-M05	4
Fagron	Eosina amarela	14H28-M09	2
Fagron	Eosina amarela	15G01-T03	1
Fagron	Eosina amarela	15G01-T03-025958	5
Fagron	Eosina amarela	15G01T03025959	1
Fagron	Eosina amarela	15G01-T03-027933	2
Fagron	Eosina amarela	15G01-T03-034438	1
Fagron	Eosina amarela	17372-87-1	2
Fagron	Eosina amarela	17K21-T0-054710	1
Fagron	Eosina amarela	17K21-T07	4
Fagron	Eosina amarela	17K21-T07_062160	1
Fagron	Eosina amarela	17K21-T07-042542	4
Fagron	Eosina amarela	17K21T07-054710	1
Fagron	Eosina amarela	17K21-T07-054710	9
Fagron	Eosina amarela	17K21-T07-057542	4
Fagron	Eosina amarela	17K21-T07-057543	1
Fagron	Eosina amarela	17K21T07060102	1
Fagron	Eosina amarela	17K21-T07-060102	7
Fagron	Eosina amarela	17K21-T07-060103	1
Fagron	Eosina amarela	17K21-T07-062160	14
Fagron	Eosina amarela	19j25-b06-196532	2
Fagron	Eosina amarela	19J25-B06-196532	10
Fagron	Eosina amarela	201856	1
Fagron	Eosina amarela	20g07-b02-200510	1
Fagron	Eosina amarela	20G07-B02-200510	7
Fagron	Eosina amarela	20G07-B02-200567	1
Fagron	Eosina amarela	20J13_B01_201856	1
Fagron	Eosina amarela	20J13-B01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eosina amarela	20J13-B01-201856	19
Fagron	Eosina amarela	20J13-B01	1
Fagron	Eosina amarela	20J13-B01-201856	1
Fagron	Eosina amarela	21L20-B06	1
Fagron	Eosina amarela	21L20-B06-213987	7
Fagron	Eosina amarela	2200510	1
Fagron	Eosina amarela	54710	1
Fagron	Eosina amarela	701074-0001	1
Fagron	Eosina amarela	B01-2018506	1
Fagron	Eosina amarela	B06-1965302	5
Fagron	Eosina amarela	EYWS/02/20	1
Fagron	Eosina amarela	EYWS/09/17	1
Fagron	Eosina amarela	EYWS/12/19	2
Fagron	Eosina amarela	EYWS/15/13	1
Fagron	Eosina amarela	EYWS/16/11	2
Fagron	Eosina amarela	EYWS/16/9	1
Fagron	Eosina amarela	T07-0621600	1
Fargon/noweda	Eosina amarela	21L20-B06-213987	1
Fargon/Sanacorp	Eosina amarela	13/11-No3	1
Fargon	Eosina amarela	19J25-B06-196532	2
Fiebig	Eosina amarela	13F14-T01-017395	1
Fiebig	Eosina amarela	EYWS/16/19	1
Gehe	Eosina amarela	14H28-M05	1
Gehe	Eosina amarela	19j25-b06-196532	1
Gehe	Eosina amarela	20J13-B01-201856	1
Gilbert/Gehe	Eosina amarela	1K21-T07-062160	1
JPN Pharma Pvt Ltd	Eosina amarela	21L20-B06	1
L12	Eosina amarela	17K21-T07-054710	1
Noweda	Eosina amarela	20J13B01201856	1
Noweda	Eosina amarela	21L20-B06	1
Sanacorp	Eosina amarela	12E25-N01	1
sanacorp	Eosina amarela	14H28-M05	1
Sanacorp	Eosina amarela	22127-B01-223849	1
Sanacorp	Eosina amarela	T07-0621600	1

- 235 867 spectra from 1515 *Apo-Ident* customers from a total of 49 189 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Eosina amarela* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Eosina amarela* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	200	0	201 884
Type C	0	196	4	235 867

The substance/substance group *Eosina amarela* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.0000 % (> 96.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20900	22534	57,15	187,44
22261	22261	0,00	160,87
22534	22534	0,00	152,40
22535	22660	2,20	216,27
22660	22660	0,00	217,06
22816	22816	0,00	214,49
23975	23975	0,00	165,26
25187	22660	44,99	192,94
25503	22660	76,40	206,07
26822	22534	116,61	187,39

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Eritromicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20011-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Eritromicina; Erythromycinum

Special notes

When selecting the *Eritromicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Eritromicina	9	17	908

Second-stage model

For differentiation of the substance/substance group *Eritromicina* the following second-stage model is used:

- Submodelo 07

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Eritromicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	76,24	–
⋮	⋮	⋮
Budesonida	>50	16,44
Valerato de betametasona	>50	19,99

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Eritromicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Eritromicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Eritromicina	13175601	21323	40	20130620
Caelo	Eritromicina	160792	22438	60	20160408*
Euro OTC	Eritromicina	1308016-02	21651	60	1412542
Euro OTC	Eritromicina	1508034	21890	60	20150925*
Euro OTC	Eritromicina	1607038	22832	40	20160831*
Euro OTC	Eritromicina	1705038	23438	40	20170705*
Euro OTC	Eritromicina	1811019	24420	40	20190114*
Fagron	Eritromicina	12E24-N04	21056	60	20120607
Fagron	Eritromicina	14B06-B35-290872	21669	60	20140225

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 9 reference samples from the substance/substance group *Eritromicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 502 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 840 spectra of 21 reference samples from the substance/substance group *Eritromicina*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Eritromicina	160795	22439	60
Caelo	Eritromicina	160797	22440	60
Caelo	Eritromicina	160796	22442	60
Caelo	Eritromicina	21002046	25858	50
Caelo	Eritromicina	21002044	25859	50
Caelo	Eritromicina	22001550	26629	40
Euro OTC	Eritromicina	1906032	24781	40
Euro OTC	Eritromicina	2002018	25121	40
Euro OTC	Eritromicina	2002038	25123	40
Euro OTC	Eritromicina	2007017	25432	40
Euro OTC	Eritromicina	2010015	25574	40
Euro OTC	Eritromicina	2010014	25575	40
Euro OTC	Eritromicina	2206001	26206	40
Euro OTC	Eritromicina	2301053	26602	40
Euro OTC	Eritromicina	2308010	26940	40
Euro OTC	Eritromicina	2407014	27369	40
Fagron	Eritromicina	23D27-B01-227928	26824	40
Caelo	Eritromicina	22001550	26629SI	20
Euro OTC	Eritromicina	2206001	26206SI	20
Euro OTC	Eritromicina	2301053	26602SI	20
Euro OTC	Eritromicina	2407014	27369SI	20

- 201 244 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6320 spectra from 1306 *Apo-Ident* customers from 956 batches from the substance/substance group *Eritromicina*.

- Among them are spectra of independent samples from 905 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Eritromicina		1
	Eritromicina	1308016-02	1
	Eritromicina	2007017-01	2
	Eritromicina	2010015-03	1
	Eritromicina	21/13-B02-213864	1
	Eritromicina	21002041006	1
	Eritromicina	21002041007	1
	Eritromicina	21002041009	1
	Eritromicina	21002041010	3
	Eritromicina	21002041011	2
	Eritromicina	21002041014	3
	Eritromicina	21002042001	1
	Eritromicina	21002053002	6
	Eritromicina	2113-B02-213864	1
	Eritromicina	21A26-F01-376732	3
	Eritromicina	21F02-F02-379295	1
	Eritromicina	21I13-B02-213865	5
	Eritromicina	21l13-B02-213865	1
	Eritromicina	22001550001	3
	Eritromicina	22001550002	7
	Eritromicina	22001550003	5
	Eritromicina	22001550005	10
	Eritromicina	22002199001	7
	Eritromicina	22002199002	7
	Eritromicina	22002199003	2
	Eritromicina	22002200001	2
	Eritromicina	22002200002	3
	Eritromicina	22002200003	3
	Eritromicina	22002200004	9
	Eritromicina	22002200005	4
	Eritromicina	22002202003	6
	Eritromicina	22002203001	1
	Eritromicina	2206001-01	13
	Eritromicina	2208001-01	1
	Eritromicina	221/13-B02-213770	1
	Eritromicina	2-21386004	1
	Eritromicina	22C2200P	1
	Eritromicina	22C2300P	1
	Eritromicina	22C230P	2
	Eritromicina	23003351002	1
	Eritromicina	23003387001	1
	Eritromicina	23003387002	1
	Eritromicina	2301052-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Eritromicina	230105301	1
	Eritromicina	2301053-01	26
	Eritromicina	2301053-02	11
	Eritromicina	2308010-01	5
	Eritromicina	23d27_b01_227795	1
	Eritromicina	23D27-B01-227795	1
	Eritromicina	23D27-B01-227928	2
	Eritromicina	23D27-B01-227929	7
	Eritromicina	23D27-B01-227930	1
	Eritromicina	23H23-B04-231446	2
	Eritromicina	324464	1
	Eritromicina	4H21P	2
	Eritromicina	A000586(Campus)	1
	Eritromicina	B01-2277905	1
	Eritromicina	B01-2279300	2
	Eritromicina	B01-2279301	1
	Eritromicina	B34-0011103	1
	Eritromicina	CEPEB004H21P	1
	Eritromicina	CEPEB022C22P	1
,0+	Eritromicina	180964001	1
AbZ	Eritromicina	18F05-B01-350908	1
AHC 04.07.13 EK38,50	Eritromicina	12156207	1
AHD 26.02.16 13,15EUR	Eritromicina	14I30-B01-308789	1
AHD/EuRho	Eritromicina	1906032-01	1
AHD	Eritromicina	1409019-02	1
AHD	Eritromicina	180964005	1
AHD	Eritromicina	18110119-01	1
AHD	Eritromicina	21002041002	1
AHD	Eritromicina	22001550002	1
AHD	Eritromicina	22002199001	2
AHD	Eritromicina	22002200005	2
AHD	Eritromicina	2301053-01	1
AHD	Eritromicina	2301053-02	1
AHD	Eritromicina	2308010-01	1
AlH	Eritromicina	15042902	1
Alliance Health	Eritromicina	120503502	1
Alliance Healthcare	Eritromicina	12E24-N04	1
Alliance Healthcare	Eritromicina	13F12-N21	1
Alliance Healthcare	Eritromicina	1607038-02	1
Alliance healthcare	Eritromicina	20003732007	1
Alliance Healthcare	Eritromicina	20E18-F06-371571	1
Alliance Healthcare	Eritromicina	21002041006	1
Alliance Healthcare	Eritromicina	21A26-F01-376731	5
Alliance Healthcare	Eritromicina	22002200004	1
Alliance Healthcare	Eritromicina	CEPEB003D20P	1
Alliance	Eritromicina	22001550002	1
Alliance	Eritromicina	2206001-01	1
alliance	Eritromicina	2301053-01	1
Allianz Healthcare	Eritromicina	16079602	1
Allianz Healthcare	Eritromicina	1811019-02	1
Alte Apotheke	Eritromicina	16079206	1
Anuh Pharma Itd (site)	Eritromicina	20I07-F06-375516	1
Anuh Pharma Itd/ AHD	Eritromicina	19C21-B03-361400	1
Anuh Pharma Itd/ AHD	Eritromicina	19C21-B03-361725	1
Anuh Pharma Itd/ AHD	Eritromicina	19C-B03-361400	1
Anuh Pharma/Sanacorp	Eritromicina	19L18-F02-3677709	1
Anuh Pharma	Eritromicina	18Fo5-B01-354817	1
Anzag 23.11.12 ek:26,49	Eritromicina	1205035-01	1
Anzag	Eritromicina	12152206	1
Anzag	Eritromicina	13175506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Eritromicina	14044001	1
Anzag	Eritromicina	16079501	1
Anzag	Eritromicina	2010014-01	1
Anzag	Eritromicina	22002199001	1
Apo-Ident / Phoenix	Eritromicina	EBS/1701-BM-001	1
Apoident/ Phoenix	Eritromicina	1906032-01	1
apo-ident/Alliance	Eritromicina	2007017-01	1
apo-ident/GEHE	Eritromicina	1607038-01	4
apo-ident/Phoenix	Eritromicina	190292002	1
apo-ident/Phönix	Eritromicina	2010014-01	1
apo-ident/Phönix	Eritromicina	2010015-01	1
apo-ident	Eritromicina	1607038-01	1
apo-ident	Eritromicina	1607038-02	1
apo-ident	Eritromicina	1705038-01	1
Audor Pharma	Eritromicina	13175602	1
Audor Pharma	Eritromicina	2002018-01	1
Audor Pharma	Eritromicina	2010015-01	1
Audor Pharma	Eritromicina	APEB022/17E	1
Audor Pharma	Eritromicina	APEB022I17E	1
Audor Pharma	Eritromicina	EB022I17E	1
Biomed / Gehe	Eritromicina	1508034-01	1
Biomed / Gehe	Eritromicina	1508034-02	1
Biomed / Gehe	Eritromicina	1705038-03	1
Biomed/Phönix	Eritromicina	1607038-01	1
Biomed	Eritromicina	1508035-01	1
Bionorica Ethics	Eritromicina	1906032-01EBS/19-022	1
Bombastus	Eritromicina	14B06-B35-290873	1
Bombastus	Eritromicina	14F13-B02	1
Bombastus	Eritromicina	15042603	1
Bombastus	Eritromicina	16079606	1
Bombastus	Eritromicina	1705038-03	1
Bombastus	Eritromicina	17088402	1
Caelo	Eritromicina		4
Caelo	Eritromicina	10079203	1
Caelo	Eritromicina	1008018-02	1
Caelo	Eritromicina	10091502	1
Caelo	Eritromicina	10788402	1
Caelo	Eritromicina	10896403	1
Caelo	Eritromicina	1091801	1
Caelo	Eritromicina	1102024-01	1
Caelo	Eritromicina	11092001	1
Caelo	Eritromicina	1114Q-01362	1
Caelo	Eritromicina	11195306	1
Caelo	Eritromicina	11195402	3
Caelo	Eritromicina	11195405	1
Caelo	Eritromicina	11195407	3
Caelo	Eritromicina	11195408	1
Caelo	Eritromicina	1171116	1
Caelo	Eritromicina	1181116	1
Caelo	Eritromicina	1195407	1
Caelo	Eritromicina	11j06-n05	1
Caelo	Eritromicina	1205036-01	2
Caelo	Eritromicina	12051801	1
Caelo	Eritromicina	12152101	3
Caelo	Eritromicina	12152102	3
Caelo	Eritromicina	12152104	2
Caelo	Eritromicina	12152105	3
Caelo	Eritromicina	12152107	1
Caelo	Eritromicina	12152108	3
Caelo	Eritromicina	12152109	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	1215219	1
Caelo	Eritromicina	12152201	8
Caelo	Eritromicina	12152202	3
Caelo	Eritromicina	12152203	1
Caelo	Eritromicina	12152205	10
Caelo	Eritromicina	12152206	9
Caelo	Eritromicina	12152208	4
Caelo	Eritromicina	12156201	3
Caelo	Eritromicina	12156202	7
Caelo	Eritromicina	12156203	2
Caelo	Eritromicina	12156204	4
Caelo	Eritromicina	12156206	2
Caelo	Eritromicina	12156207	3
Caelo	Eritromicina	12156208	6
Caelo	Eritromicina	12E24-N04	1
Caelo	Eritromicina	13011810	1
Caelo	Eritromicina	1308016-01	2
Caelo	Eritromicina	1308016-02	1
Caelo	Eritromicina	13145504	1
Caelo	Eritromicina	1315501	1
Caelo	Eritromicina	13175501	6
Caelo	Eritromicina	13175502	4
Caelo	Eritromicina	13175503	8
Caelo	Eritromicina	13175504	6
Caelo	Eritromicina	13175504-3413310132	1
Caelo	Eritromicina	13175505	4
Caelo	Eritromicina	13175506	4
Caelo	Eritromicina	13175506-3559412014	1
Caelo	Eritromicina	13175601	10
Caelo	Eritromicina	131756017	1
Caelo	Eritromicina	13175603	11
Caelo	Eritromicina	13175604	7
Caelo	Eritromicina	13175607	8
Caelo	Eritromicina	13175608	6
Caelo	Eritromicina	13175610	1
Caelo	Eritromicina	13175611	5
Caelo	Eritromicina	13175612	2
Caelo	Eritromicina	13175801	10
Caelo	Eritromicina	13175802	8
Caelo	Eritromicina	13175803	8
Caelo	Eritromicina	13175804	2
Caelo	Eritromicina	13175808	2
Caelo	Eritromicina	13175809	5
Caelo	Eritromicina	13175810	4
Caelo	Eritromicina	13175811	8
Caelo	Eritromicina	13178756tzgklhj	1
Caelo	Eritromicina	13189001	8
Caelo	Eritromicina	13189002	7
Caelo	Eritromicina	13189004	5
Caelo	Eritromicina	13189006	3
Caelo	Eritromicina	13189007	2
Caelo	Eritromicina	132152108	1
Caelo	Eritromicina	13A02-N06	1
Caelo	Eritromicina	13D30-N01	3
Caelo	Eritromicina	13H22-N07	1
Caelo	Eritromicina	14/30-B01-300059	1
Caelo	Eritromicina	14/30-B01-308189	2
Caelo	Eritromicina	140044203	1
Caelo	Eritromicina	140440006	1
Caelo	Eritromicina	14044001	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	14044002	10
Caelo	Eritromicina	14044004	11
Caelo	Eritromicina	140440044	1
Caelo	Eritromicina	14044005	11
Caelo	Eritromicina	14044006	6
Caelo	Eritromicina	14044007	8
Caelo	Eritromicina	14044008	4
Caelo	Eritromicina	14044009	3
Caelo	Eritromicina	14044010	4
Caelo	Eritromicina	14044011	2
Caelo	Eritromicina	14044012	3
Caelo	Eritromicina	14044014	3
Caelo	Eritromicina	1404409	1
Caelo	Eritromicina	14044101	7
Caelo	Eritromicina	14044105	4
Caelo	Eritromicina	14044106	3
Caelo	Eritromicina	14044107	3
Caelo	Eritromicina	14044109	5
Caelo	Eritromicina	14044110	1
Caelo	Eritromicina	14044114	6
Caelo	Eritromicina	14044115	6
Caelo	Eritromicina	14044118	3
Caelo	Eritromicina	1404414	1
Caelo	Eritromicina	1404418	1
Caelo	Eritromicina	14044201	5
Caelo	Eritromicina	14044202	3
Caelo	Eritromicina	14044205	4
Caelo	Eritromicina	14044206	3
Caelo	Eritromicina	14044207	2
Caelo	Eritromicina	1409019	1
Caelo	Eritromicina	1409019-01	2
Caelo	Eritromicina	140901902	2
Caelo	Eritromicina	1409019-02	4
Caelo	Eritromicina	140930E	1
Caelo	Eritromicina	1414M-01362	1
Caelo	Eritromicina	1430b01300059	1
Caelo	Eritromicina	14B06-B35-290872	1
Caelo	Eritromicina	14B06-B35-290873	1
Caelo	Eritromicina	14b06-b35-293508	1
Caelo	Eritromicina	14F13-B02-296464	2
Caelo	Eritromicina	14F13-B02-300061	1
Caelo	Eritromicina	14I30-B01	1
Caelo	Eritromicina	14I30-B01-308789	1
Caelo	Eritromicina	150242813	1
Caelo	Eritromicina	15042601	2
Caelo	Eritromicina	15042602	8
Caelo	Eritromicina	15042603	6
Caelo	Eritromicina	15042604	3
Caelo	Eritromicina	15042605	9
Caelo	Eritromicina	15042606	1
Caelo	Eritromicina	15042608	3
Caelo	Eritromicina	15042609	8
Caelo	Eritromicina	15042610	10
Caelo	Eritromicina	15042611	5
Caelo	Eritromicina	15042611-20160504Ma1	1
Caelo	Eritromicina	15042612	7
Caelo	Eritromicina	15042613	4
Caelo	Eritromicina	15042701	12
Caelo	Eritromicina	15042702	4
Caelo	Eritromicina	15042703	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	15042704	9
Caelo	Eritromicina	15042705	12
Caelo	Eritromicina	15042706	10
Caelo	Eritromicina	15042707	1
Caelo	Eritromicina	15042711	14
Caelo	Eritromicina	150427704	1
Caelo	Eritromicina	150428	1
Caelo	Eritromicina	15042802	3
Caelo	Eritromicina	15042803	14
Caelo	Eritromicina	15042804	1
Caelo	Eritromicina	15042806	12
Caelo	Eritromicina	15042808	1
Caelo	Eritromicina	15042809	3
Caelo	Eritromicina	15042810	6
Caelo	Eritromicina	15042811	3
Caelo	Eritromicina	15042812	1
Caelo	Eritromicina	15042813	14
Caelo	Eritromicina	15042814	11
Caelo	Eritromicina	15042815	3
Caelo	Eritromicina	15042816	7
Caelo	Eritromicina	15042901	10
Caelo	Eritromicina	15042902	2
Caelo	Eritromicina	1504812	1
Caelo	Eritromicina	1504813	1
Caelo	Eritromicina	150803401	1
Caelo	Eritromicina	1508034-01	1
Caelo	Eritromicina	1508034-02	3
Caelo	Eritromicina	1524002	1
Caelo	Eritromicina	1524004	1
Caelo	Eritromicina	15245002	20
Caelo	Eritromicina	15245003	9
Caelo	Eritromicina	15245004	13
Caelo	Eritromicina	15245005	2
Caelo	Eritromicina	15245007	3
Caelo	Eritromicina	15245008	3
Caelo	Eritromicina	15245008I-041016-3	1
Caelo	Eritromicina	15245101	11
Caelo	Eritromicina	154042602	1
Caelo	Eritromicina	16/24-B10-341876	1
Caelo	Eritromicina	16017088303	1
Caelo	Eritromicina	1607038	1
Caelo	Eritromicina	160703801	2
Caelo	Eritromicina	1607038-01	4
Caelo	Eritromicina	1607038-02	10
Caelo	Eritromicina	16073038-02	1
Caelo	Eritromicina	160738-01	1
Caelo	Eritromicina	16076903	1
Caelo	Eritromicina	16079201	10
Caelo	Eritromicina	16079202	12
Caelo	Eritromicina	16079203	21
Caelo	Eritromicina	16079204	14
Caelo	Eritromicina	16079205	5
Caelo	Eritromicina	16079206	5
Caelo	Eritromicina	16079207	8
Caelo	Eritromicina	16079208	9
Caelo	Eritromicina	16079209	1
Caelo	Eritromicina	16079210	9
Caelo	Eritromicina	16079213	14
Caelo	Eritromicina	16079214	11
Caelo	Eritromicina	16079214-20170704Ma1	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	16079214-20171127Ma6	1
Caelo	Eritromicina	16079214-24417/1	1
Caelo	Eritromicina	16079216	8
Caelo	Eritromicina	16079501	20
Caelo	Eritromicina	16079502	15
Caelo	Eritromicina	16079503	8
Caelo	Eritromicina	16079505	3
Caelo	Eritromicina	16079506	7
Caelo	Eritromicina	16079507	1
Caelo	Eritromicina	16079509	29
Caelo	Eritromicina	16079510	9
Caelo	Eritromicina	16079511	10
Caelo	Eritromicina	16079512	5
Caelo	Eritromicina	16079513	11
Caelo	Eritromicina	16079514	1
Caelo	Eritromicina	16079515	1
Caelo	Eritromicina	160796	1
Caelo	Eritromicina	16079602	5
Caelo	Eritromicina	16079603	15
Caelo	Eritromicina	16079604	5
Caelo	Eritromicina	16079605	2
Caelo	Eritromicina	16079606	7
Caelo	Eritromicina	16079607	1
Caelo	Eritromicina	16079608	21
Caelo	Eritromicina	16079609	8
Caelo	Eritromicina	16079610	1
Caelo	Eritromicina	16079612	16
Caelo	Eritromicina	16079613	2
Caelo	Eritromicina	16079614	6
Caelo	Eritromicina	16079701	1
Caelo	Eritromicina	16079702	8
Caelo	Eritromicina	16079704	4
Caelo	Eritromicina	16091712	1
Caelo	Eritromicina	16979201	1
Caelo	Eritromicina	16G06-803	1
Caelo	Eritromicina	16G06-B03-324463	1
Caelo	Eritromicina	16G06-B03-324464	3
Caelo	Eritromicina	16G06-B03-324465	1
Caelo	Eritromicina	16G06-B03-324466	2
Caelo	Eritromicina	16G06B03329150	1
Caelo	Eritromicina	16G06-B03-329150	1
Caelo	Eritromicina	16i24-B10	1
Caelo	Eritromicina	16j24b1033673	1
Caelo	Eritromicina	16J24-B10-339487	1
Caelo	Eritromicina	16J24-B10-341875	1
Caelo	Eritromicina	16J24-B10-341876	1
Caelo	Eritromicina	16J24-B-341876	1
Caelo	Eritromicina	1705037-01	1
Caelo	Eritromicina	1705038	2
Caelo	Eritromicina	1705038_02	1
Caelo	Eritromicina	170503801	1
Caelo	Eritromicina	1705038-01	7
Caelo	Eritromicina	170503802	1
Caelo	Eritromicina	1705038-02	4
Caelo	Eritromicina	1705038-03	2
Caelo	Eritromicina	17068309	1
Caelo	Eritromicina	170718A	1
Caelo	Eritromicina	1708/8308	1
Caelo	Eritromicina	17086301	1
Caelo	Eritromicina	17088001	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	17088002	19
Caelo	Eritromicina	17088003	12
Caelo	Eritromicina	17088004	14
Caelo	Eritromicina	17088005	14
Caelo	Eritromicina	17088007	11
Caelo	Eritromicina	17088008	15
Caelo	Eritromicina	17088008-20180206Ma2	1
Caelo	Eritromicina	17088008-E20180112Ma	1
Caelo	Eritromicina	17088009	11
Caelo	Eritromicina	17088010	14
Caelo	Eritromicina	17088010-20180404Ma2	1
Caelo	Eritromicina	170880103	1
Caelo	Eritromicina	17088011	1
Caelo	Eritromicina	17088013	35
Caelo	Eritromicina	17088013/1250418	1
Caelo	Eritromicina	1708807	1
Caelo	Eritromicina	1708808	2
Caelo	Eritromicina	17088203	19
Caelo	Eritromicina	17088204	48
Caelo	Eritromicina	17088206	1
Caelo	Eritromicina	17088207	9
Caelo	Eritromicina	17088208	2
Caelo	Eritromicina	17088210	34
Caelo	Eritromicina	17088210-E20181115Ma	1
Caelo	Eritromicina	17088212	1
Caelo	Eritromicina	17088301	70
Caelo	Eritromicina	17088302	4
Caelo	Eritromicina	17088303	7
Caelo	Eritromicina	17088304	1
Caelo	Eritromicina	17088305	28
Caelo	Eritromicina	17088305031110172	1
Caelo	Eritromicina	17088306	38
Caelo	Eritromicina	17088308	12
Caelo	Eritromicina	17088309	22
Caelo	Eritromicina	17088401	8
Caelo	Eritromicina	17088402	17
Caelo	Eritromicina	17088403	25
Caelo	Eritromicina	17088403-20180619Ma1	1
Caelo	Eritromicina	17088403-E2081115Ma1	1
Caelo	Eritromicina	17088404	25
Caelo	Eritromicina	17088405	19
Caelo	Eritromicina	17088406	11
Caelo	Eritromicina	170888309	1
Caelo	Eritromicina	1709038-01	1
Caelo	Eritromicina	17219705	1
Caelo	Eritromicina	1780210	1
Caelo	Eritromicina	178824	1
Caelo	Eritromicina	1788402	1
Caelo	Eritromicina	180096302	1
Caelo	Eritromicina	18094606	1
Caelo	Eritromicina	18095303	1
Caelo	Eritromicina	1809604	1
Caelo	Eritromicina	180960405	1
Caelo	Eritromicina	18096201	25
Caelo	Eritromicina	180962011905013-04	1
Caelo	Eritromicina	18096202	14
Caelo	Eritromicina	18096203	1
Caelo	Eritromicina	18096204	5
Caelo	Eritromicina	18096205	26
Caelo	Eritromicina	18096206	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	18096207	2
Caelo	Eritromicina	18096208	17
Caelo	Eritromicina	18096209	29
Caelo	Eritromicina	18096210	12
Caelo	Eritromicina	18096211	10
Caelo	Eritromicina	1809630	1
Caelo	Eritromicina	18096302	19
Caelo	Eritromicina	18096303	15
Caelo	Eritromicina	18096304	5
Caelo	Eritromicina	18096305	3
Caelo	Eritromicina	180964001	27
Caelo	Eritromicina	180964002	7
Caelo	Eritromicina	180964003	15
Caelo	Eritromicina	180964004	4
Caelo	Eritromicina	180964005	4
Caelo	Eritromicina	18096401	33
Caelo	Eritromicina	18096403	13
Caelo	Eritromicina	18096404	9
Caelo	Eritromicina	18096405	24
Caelo	Eritromicina	18096406	30
Caelo	Eritromicina	180964403	1
Caelo	Eritromicina	1811019-01	6
Caelo	Eritromicina	1811019-02	1
Caelo	Eritromicina	18215001	3
Caelo	Eritromicina	18F05-B01-350907	1
Caelo	Eritromicina	18F05-B01-350908	1
Caelo	Eritromicina	18F05-B01-35096	1
Caelo	Eritromicina	18F05-B01-356705	1
Caelo	Eritromicina	18F05-B01-356706	2
Caelo	Eritromicina	18F05-B01-358087	1
Caelo	Eritromicina	19011908	1
Caelo	Eritromicina	1903060E	1
Caelo	Eritromicina	1906032-01	6
Caelo	Eritromicina	19071306	1
Caelo	Eritromicina	19096406	1
Caelo	Eritromicina	19C21B03361400	1
Caelo	Eritromicina	19L18-F02-367776	1
Caelo	Eritromicina	19L18-F02367779	1
Caelo	Eritromicina	200002258002	1
Caelo	Eritromicina	200002259007	1
Caelo	Eritromicina	200003731001	1
Caelo	Eritromicina	200003731004	1
Caelo	Eritromicina	200022259008	1
Caelo	Eritromicina	20002250002	1
Caelo	Eritromicina	20002258001	3
Caelo	Eritromicina	20002258002	20
Caelo	Eritromicina	20002258003	2
Caelo	Eritromicina	20002259002	24
Caelo	Eritromicina	20002259003	23
Caelo	Eritromicina	20002259003/4620	1
Caelo	Eritromicina	20002259004	4
Caelo	Eritromicina	20002259005	11
Caelo	Eritromicina	20002259006	26
Caelo	Eritromicina	20002259007	15
Caelo	Eritromicina	20002259008	2
Caelo	Eritromicina	20003431004	1
Caelo	Eritromicina	2000373007	1
Caelo	Eritromicina	2000373009	1
Caelo	Eritromicina	20003731001	23
Caelo	Eritromicina	20003731002	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	20003731003	25
Caelo	Eritromicina	20003731004	28
Caelo	Eritromicina	20003731005	27
Caelo	Eritromicina	20003732001	16
Caelo	Eritromicina	20003732002	7
Caelo	Eritromicina	20003732004	13
Caelo	Eritromicina	20003732005	6
Caelo	Eritromicina	20003732006	1
Caelo	Eritromicina	20003732007	11
Caelo	Eritromicina	20003732008	15
Caelo	Eritromicina	20003732009	28
Caelo	Eritromicina	20003732010	27
Caelo	Eritromicina	20003732011	3
Caelo	Eritromicina	20003733001	7
Caelo	Eritromicina	2000373731004	1
Caelo	Eritromicina	2000373732010	1
Caelo	Eritromicina	20003762010	1
Caelo	Eritromicina	20004278008	1
Caelo	Eritromicina	2002258002	1
Caelo	Eritromicina	2003731005	1
Caelo	Eritromicina	2003732011	1
Caelo	Eritromicina	2003733001	1
Caelo	Eritromicina	2007017-01	3
Caelo	Eritromicina	2010015-01	3
Caelo	Eritromicina	2010015-03	1
Caelo	Eritromicina	20122013D	1
Caelo	Eritromicina	20270912-3	1
Caelo	Eritromicina	20E18-F05-371567	1
Caelo	Eritromicina	20E18-F06	1
Caelo	Eritromicina	20E18-F06-372104	1
Caelo	Eritromicina	20I07-F06	1
Caelo	Eritromicina	2100100204	1
Caelo	Eritromicina	21002041001	8
Caelo	Eritromicina	21002041002	11
Caelo	Eritromicina	21002041003	3
Caelo	Eritromicina	21002041006	6
Caelo	Eritromicina	21002041007	13
Caelo	Eritromicina	21002041008	2
Caelo	Eritromicina	21002041009	4
Caelo	Eritromicina	21002041010	7
Caelo	Eritromicina	21002041012	1
Caelo	Eritromicina	21002041014	8
Caelo	Eritromicina	21002042001	15
Caelo	Eritromicina	21002044001	2
Caelo	Eritromicina	21002044002	3
Caelo	Eritromicina	210020441004	1
Caelo	Eritromicina	21002046001	3
Caelo	Eritromicina	21002053002	1
Caelo	Eritromicina	2100242001	1
Caelo	Eritromicina	21A26-F01	1
Caelo	Eritromicina	21A26-F01-376731	1
Caelo	Eritromicina	22001550001	3
Caelo	Eritromicina	22001550002	5
Caelo	Eritromicina	22002199001	1
Caelo	Eritromicina	22002200001	9
Caelo	Eritromicina	22002200002	4
Caelo	Eritromicina	22002200003	1
Caelo	Eritromicina	22002202001	1
Caelo	Eritromicina	22041302	1
Caelo	Eritromicina	23021710	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eritromicina	24071402	1
Caelo	Eritromicina	24101312	1
Caelo	Eritromicina	26011402	1
Caelo	Eritromicina	27071202	1
Caelo	Eritromicina	2761	1
Caelo	Eritromicina	28041505	1
Caelo	Eritromicina	28101405	1
Caelo	Eritromicina	30011505	1
Caelo	Eritromicina	308160l	1
Caelo	Eritromicina	3092014B	1
Caelo	Eritromicina	3110195	1
Caelo	Eritromicina	3317	1
Caelo	Eritromicina	4316E-01362	1
Caelo	Eritromicina	5042604	1
Caelo	Eritromicina	5052015D	1
Caelo	Eritromicina	511111	1
Caelo	Eritromicina	59/AKD59	1
Caelo	Eritromicina	60/AKD4	1
Caelo	Eritromicina	618E-01362	1
Caelo	Eritromicina	80963021	1
Caelo	Eritromicina	Caelo	1
Caelo	Eritromicina	EB06/14	1
Caelo	Eritromicina	I31032016/1	1
Caeolo/Krieger	Eritromicina	17088004	1
Caeolo/Noweda	Eritromicina	13189007	1
Caeolo/Noweda	Eritromicina	16079603	1
Caesa / Alliance Hea...	Eritromicina	17088309	1
Caesar & Lorenz GmbH	Eritromicina	15042611	1
Caesar & Loretz GmbH...	Eritromicina	20003732009	1
Caesar & Loretz GmbH...	Eritromicina	20002259003	1
Caesar & Loretz GmbH...	Eritromicina	20003731005	1
Caesar & Loretz GmbH...	Eritromicina	18096211	1
Caesar & Loretz GmbH...	Eritromicina	18096401	1
Caesar & Loretz GmbH...	Eritromicina	18096405	2
Caesar & Loretz GmbH...	Eritromicina	18096406	1
Caesar & Loretz GmbH...	Eritromicina	17088404	1
Caesar & Loretz GmbH...	Eritromicina	18096201	1
Caesar & Loretz GmbH...	Eritromicina	18096208	1
Caesar & Loretz GmbH...	Eritromicina	18096406	1
Caesar & Loretz GmbH...	Eritromicina	22001550002	1
Caesar & Loretz GmbH...	Eritromicina	20003732002	1
Caesar & Loretz GmbH...	Eritromicina	180964005	1
Caesar & Loretz GmbH...	Eritromicina	18096401	1
Caesar & Loretz GmbH...	Eritromicina	10217208	1
Caesar & Loretz GmbH...	Eritromicina	13189002	1
Caesar & Loretz GmbH...	Eritromicina	17088003	1
Caesar & Loretz GmbH...	Eritromicina	20003731001	2
Caesar & Loretz GmbH...	Eritromicina	16079207	1
Caesar & Loretz GmbH...	Eritromicina	21002041002	1
Caesar & Loretz GmbH/ G	Eritromicina	18096201	1
Caesar & Loretz GmbH...	Eritromicina	20003732010	1
Caesar & Loretz GmbH/ GTH	Eritromicina	18096209	1
Caesar & Loretz GmbH...	Eritromicina	21002041010	1
Caesar & Loretz GmbH...	Eritromicina	20003731004	3
Caesar & Loretz GmbH...	Eritromicina	180964001	1
Caesar & Loretz GmbH...	Eritromicina	20003731004	1
Caesar & Loretz GmbH/AEP	Eritromicina	18096302	2
Caesar & Loretz GmbH/AEP	Eritromicina	22002200002	1
Caesar & Loretz GmbH/AHD	Eritromicina	20002259005	1
Caesar & Loretz GmbH/AHD	Eritromicina	20003733001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Eritromicina	17088303	1
Caesar & Loretz GmbH...	Eritromicina	20003731004	1
Caesar & Loretz GmbH...	Eritromicina	20003732008	1
Caesar & Loretz GmbH...	Eritromicina	20003732010	1
Caesar & Loretz GmbH...	Eritromicina	20002259006	2
Caesar & Loretz GmbH/E	Eritromicina	21002041001	1
Caesar & Loretz GmbH...	Eritromicina	18096404	1
Caesar & Loretz GmbH...	Eritromicina	20003732007	1
Caesar & Loretz GmbH/G	Eritromicina	20002258002	1
Caesar & Loretz GmbH/Gehe	Eritromicina	18096208	1
Caesar & Loretz GmbH/Gehe	Eritromicina	18096209	1
Caesar & Loretz GmbH/Gehe	Eritromicina	180964002	1
Caesar & Loretz GmbH/Gehe	Eritromicina	18096401	1
Caesar & Loretz GmbH/Gehe	Eritromicina	18096405	1
Caesar & Loretz GmbH/Gehe	Eritromicina	18096406	3
Caesar & Loretz GmbH/Gehe	Eritromicina	22002199001	1
Caesar & Loretz GmbH...	Eritromicina	20002258003	1
Caesar & Loretz GmbH...	Eritromicina	20003732002	1
Caesar & Loretz GmbH...	Eritromicina	21002041008	1
Caesar & Loretz GmbH...	Eritromicina	20002259002	1
Caesar & Loretz GmbH...	Eritromicina	20003731004	1
Caesar & Loretz GmbH...	Eritromicina	20003732010	1
Caesar & Loretz GmbH...	Eritromicina	21002041009	1
Caesar & Loretz GmbH...	Eritromicina	18096302	1
Caesar & Loretz GmbH...	Eritromicina	20002259002	1
Caesar & Loretz GmbH...	Eritromicina	20003731004	1
Caesar & Loretz GmbH...	Eritromicina	21002041001	1
Caesar & Loretz GmbH...	Eritromicina	21002042001	1
Caesar & Loretz GmbH/Kehr	Eritromicina	F05-3715605	1
Caesar & Loretz GmbH...	Eritromicina	20003731003	1
Caesar & Loretz GmbH...	Eritromicina	200201801	1
Caesar & Loretz GmbH...	Eritromicina	18096405	1
Caesar & Loretz GmbH...	Eritromicina	20002259007	1
Caesar & Loretz GmbH...	Eritromicina	20003731001	1
Caesar & Loretz GmbH...	Eritromicina	20003732008	1
Caesar & Loretz GmbH...	Eritromicina	21002041002	1
Caesar & Loretz GmbH/Ph	Eritromicina	1906032-01	1
Caesar & Loretz GmbH/Phoe	Eritromicina	20002258003	1
Caesar & Loretz GmbH...	Eritromicina	22002199001	1
Caesar & Loretz GmbH...	Eritromicina	180964003	2
Caesar & Loretz GmbH...	Eritromicina	20002259003	1
Caesar & Loretz GmbH...	Eritromicina	20002259005	1
Caesar & Loretz GmbH...	Eritromicina	20002259007	1
Caesar & Loretz GmbH...	Eritromicina	20003731005	1
Caesar & Loretz GmbH...	Eritromicina	20003732007	1
Caesar & Loretz GmbH...	Eritromicina	20003732008	1
Caesar & Loretz GmbH...	Eritromicina	20003732009	2
Caesar & Loretz GmbH...	Eritromicina	18096209	1
Caesar & Loretz GmbH...	Eritromicina	180964001	1
Caesar & Loretz GmbH...	Eritromicina	18096403	1
Caesar & Loretz GmbH...	Eritromicina	20002258002	1
Caesar & Loretz GmbH...	Eritromicina	20002259003	1
Caesar & Loretz GmbH...	Eritromicina	20003732008	1
Caesar & Loretz GmbH...	Eritromicina	20003732009	1
Caesar & Loretz GmbH...	Eritromicina	21002041002	2
Caesar & Loretz GmbH...	Eritromicina	21002041006	1
Caesar & Loretz GmbH...	Eritromicina	21002041007	2
Caesar & Loretz GmbH...	Eritromicina	21002042001	1
Caesar & Loretz GmbH...	Eritromicina	AP220827-07	1
Caesar & Loretz GmbH...	Eritromicina	21002044001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Wepa	Eritromicina	180964003	1
Caesar & Loretz GmbH	Eritromicina	15042814	1
Caesar & Loretz GmbH	Eritromicina	16079509	2
Caesar & Loretz GmbH	Eritromicina	17088005	1
Caesar & Loretz GmbH	Eritromicina	17088305	2
Caesar & Loretz GmbH	Eritromicina	17088306	6
Caesar & Loretz GmbH	Eritromicina	17088308	1
Caesar & Loretz GmbH	Eritromicina	17088309	8
Caesar & Loretz GmbH	Eritromicina	17088403	1
Caesar & Loretz GmbH	Eritromicina	17088404	2
Caesar & Loretz GmbH	Eritromicina	18096201	2
Caesar & Loretz GmbH	Eritromicina	18096203	1
Caesar & Loretz GmbH	Eritromicina	18096204	3
Caesar & Loretz GmbH	Eritromicina	18096205	5
Caesar & Loretz GmbH	Eritromicina	18096207	1
Caesar & Loretz GmbH	Eritromicina	18096208	3
Caesar & Loretz GmbH	Eritromicina	18096209	8
Caesar & Loretz GmbH	Eritromicina	18096210	6
Caesar & Loretz GmbH	Eritromicina	18096211	3
Caesar & Loretz GmbH	Eritromicina	18096302	2
Caesar & Loretz GmbH	Eritromicina	18096303	1
Caesar & Loretz GmbH	Eritromicina	18096304	1
Caesar & Loretz GmbH	Eritromicina	18096305	2
Caesar & Loretz GmbH	Eritromicina	180964001	2
Caesar & Loretz GmbH	Eritromicina	180964002	2
Caesar & Loretz GmbH	Eritromicina	180964003	8
Caesar & Loretz GmbH	Eritromicina	180964005	2
Caesar & Loretz GmbH	Eritromicina	18096401	18
Caesar & Loretz GmbH	Eritromicina	18096403	6
Caesar & Loretz GmbH	Eritromicina	18096404	1
Caesar & Loretz GmbH	Eritromicina	18096405	6
Caesar & Loretz GmbH	Eritromicina	18096406	6
Caesar & Loretz GmbH	Eritromicina	20002258002	1
Caesar & Loretz GmbH	Eritromicina	20002259002	4
Caesar & Loretz GmbH	Eritromicina	20002259003	7
Caesar & Loretz GmbH	Eritromicina	20002259005	4
Caesar & Loretz GmbH	Eritromicina	20002259006	8
CAESAR & LORETZ GMBH	Eritromicina	20002259006	2
Caesar & Loretz GmbH	Eritromicina	20002259007	4
Caesar & Loretz GmbH	Eritromicina	20002259008	1
Caesar & Loretz GmbH	Eritromicina	20003731001	10
Caesar & Loretz GmbH	Eritromicina	20003731002	1
Caesar & Loretz GmbH	Eritromicina	20003731003	6
Caesar & Loretz GmbH	Eritromicina	20003731004	6
Caesar & Loretz GmbH	Eritromicina	20003731005	10
Caesar & Loretz GmbH	Eritromicina	20003732001	3
Caesar & Loretz GmbH	Eritromicina	20003732002	1
Caesar & Loretz GmbH	Eritromicina	20003732004	2
Caesar & Loretz GmbH	Eritromicina	20003732007	9
Caesar & Loretz GmbH	Eritromicina	20003732008	17
Caesar & Loretz GmbH	Eritromicina	20003732009	7
Caesar & Loretz GmbH	Eritromicina	20003732010	14
Caesar & Loretz GmbH	Eritromicina	20003732011	1
Caesar & Loretz GmbH	Eritromicina	20003733001	8
Caesar & Loretz GmbH	Eritromicina	2002259005	2
Caesar & Loretz GmbH	Eritromicina	21002041002	8
Caesar & Loretz GmbH	Eritromicina	21002041003	4
Caesar & Loretz GmbH	Eritromicina	21002041004	5
Caesar & Loretz GmbH	Eritromicina	21002041008	1
Caesar & Loretz GmbH	Eritromicina	21002041009	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Eritromicina	21002041010	2
Caesar & Loretz GmbH	Eritromicina	21002041011	1
Caesar & Loretz GmbH	Eritromicina	21002041012	2
Caesar & Loretz GmbH	Eritromicina	21002041014	1
Caesar & Loretz GmbH	Eritromicina	21002042001	6
Caesar & Loretz GmbH	Eritromicina	21002044001	1
Caesar & Loretz GmbH	Eritromicina	21002046001	2
Caesar & Loretz GmbH	Eritromicina	22001550001	1
Caesar & Loretz GmbH	Eritromicina	22001550003	1
Caesar & Loretz GmbH	Eritromicina	22002200001	1
Caesar & Loretz GmbH	Eritromicina	2206001-01	1
Caesar & Loretz GmbH	Eritromicina	F02-3677709	3
Caesar & Loretz Hild...	Eritromicina	180964001	1
Caesar & Loretz Hilden	Eritromicina	17088305	1
Caesar & Loretz Hilden	Eritromicina	18096208	1
Caesar & Loretz/AHC	Eritromicina	15042813	1
Caesar & Loretz/AHD	Eritromicina	20002258002	1
Caesar & Loretz/Phönix	Eritromicina	20003732004	1
Caesar & Loretz/Sanacorp	Eritromicina	18096201	2
Caesar / Gehe	Eritromicina	15042705	1
Caesar / Gehe	Eritromicina	17088402	1
Caesar u. Loretz/Noweda	Eritromicina	16079209	1
Caesar und Loretz	Eritromicina	17088210	1
Caesar& Loretz GmbH	Eritromicina	17088305	1
Caesar&Lorenz/AHD	Eritromicina	18096303	1
Caesar&Loretz GmbH /Anzag	Eritromicina	15042610	1
Caesar&Loretz GmbH	Eritromicina	15042807	1
Caesar&Loretz GmbH	Eritromicina	20002259001	1
Caesar&Loretz GmbH	Eritromicina	21002044002	1
Caesar&loretz,Phoenix	Eritromicina	13175602	1
Caesar&loretz,Phoenix	Eritromicina	14044004	1
caesar&loretz,phönix	Eritromicina	15042603	1
Caesar/Loretz/Noweda	Eritromicina	15042610	1
Calo/AHD	Eritromicina	15042605	1
Cealo / Noweda	Eritromicina	1205036-02	1
Cealo/ Anzag	Eritromicina	16079603	2
Cealo/ Phoenix	Eritromicina	17088210	1
Cealo/Alliance Healthcare	Eritromicina	17088309	1
Cealo/Sanacorp	Eritromicina	180964003	1
Cealo	Eritromicina	16079513	1
Celo/Kehr	Eritromicina	16079608	1
Ebert & Jacobi	Eritromicina	15042611	1
Ebert & Jacobi	Eritromicina	15245007	1
Eigenherstellung	Eritromicina	14044006	1
EuRho / 2	Eritromicina	1811019-01	2
EuRho / Alliance	Eritromicina	2007017-01	1
EuRho / Noweda	Eritromicina	700770	1
EuRho 08.08.2013Alli...	Eritromicina	1205036-01	1
EuRho/ AHD	Eritromicina	1705038-01	1
EuRho/ Anzag	Eritromicina	211124(2010014-01)	1
EuRho/ NOWEDA	Eritromicina	1906032-01	1
EuRho/ Noweda	Eritromicina	2010015-02	1
EuRho/Gehe	Eritromicina	1409019-01	1
EuRho/Gehe	Eritromicina	1811019-01	1
EuRho/Gehe	Eritromicina	1906032-01	1
EuRho/Gehe	Eritromicina	2010014-01	1
EuRho/Noweda	Eritromicina	1508034-02	1
EuRho/Noweda	Eritromicina	1705038-01	1
EuRho/Noweda	Eritromicina	2002018-01	1
EuRho/Noweda	Eritromicina	2206001-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Phoenix	Eritromicina	2206001-01	2
EuRho/Phönix	Eritromicina	1106036-05	1
EuRho/Phönix	Eritromicina	1205035	1
EuRho/Phönix	Eritromicina	1308016-02	1
EuRho/Phönix	Eritromicina	1811019-01	1
EuRho/Phönix	Eritromicina	2002018-01	1
Eurho/Phönix	Eritromicina	2010014-02	1
EuRho/Sanacorp	Eritromicina	2010014-01	1
EuRho/Sanacorp	Eritromicina	2301053-01	1
EuRho	Eritromicina	1205035-01	1
EuRho	Eritromicina	1205035-02	1
EuRho	Eritromicina	1205036-01	1
EuRho	Eritromicina	1308016-02	3
EuRho	Eritromicina	1705038-01	1
EuRho	Eritromicina	1705038-02	1
EuRho	Eritromicina	1705038-03	1
EuRho	Eritromicina	1811019-01	2
EuRho	Eritromicina	1906032-01	1
EuRho	Eritromicina	2002018-01	1
EuRho	Eritromicina	2007017-01	2
EuRho	Eritromicina	2010014-02	1
Eurho	Eritromicina	2010015-01	1
EuRho	Eritromicina	2010015-01	1
EuRho	Eritromicina	2010015-03	2
Euro CT Phönix	Eritromicina	13175604	1
Euro OCT / Krieger	Eritromicina	2007017-01	1
Euro OCT / Krieger	Eritromicina	2010014-01	1
Euro Oct/Phoenix	Eritromicina	1705038-03	1
EURO OGT / Anzag	Eritromicina	1409019-01	1
Euro OT	Eritromicina	1409019-02	1
Euro OTC	Eritromicina	100(2002018-01)	1
Euro OTC	Eritromicina	101(2007017-01)	1
Euro OTC	Eritromicina	1013u-01362	1
Euro OTC	Eritromicina	1106036-04	1
Euro OTC	Eritromicina	1106036-05	6
Euro OTC	Eritromicina	111811019-02	1
Euro OTC	Eritromicina	1205035-01	13
Euro OTC	Eritromicina	120503502	1
Euro OTC	Eritromicina	1205035-02	17
Euro OTC	Eritromicina	1205036/02	1
Euro OTC	Eritromicina	120503601	1
Euro OTC	Eritromicina	1205036-01	7
Euro OTC	Eritromicina	120503602	2
Euro OTC	Eritromicina	1205036-02	9
Euro OTC	Eritromicina	12A02-N06	1
Euro OTC	Eritromicina	130801601	6
Euro OTC	Eritromicina	1308016-01	28
Euro OTC	Eritromicina	130801602	2
Euro OTC	Eritromicina	1308016-02	26
Euro OTC	Eritromicina	13175505	1
Euro OTC	Eritromicina	14044205	1
Euro OTC	Eritromicina	140901901	3
Euro OTC	Eritromicina	1409019-01	30
Euro OTC	Eritromicina	1409019-01Mg100g	1
Euro OTC	Eritromicina	140901902	1
Euro OTC	Eritromicina	1409019-02	53
Euro OTC	Eritromicina	1409019-02Gehe	1
Euro OTC	Eritromicina	14090-9-01	1
Euro OTC	Eritromicina	140919-02	2
Euro OTC	Eritromicina	15042810	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Eritromicina	15080-01	1
Euro OTC	Eritromicina	1508034	1
Euro OTC	Eritromicina	150803401	1
Euro OTC	Eritromicina	1508034-01	37
Euro OTC	Eritromicina	1508034-02	18
Euro OTC	Eritromicina	1508034-02Mg100g	1
Euro OTC	Eritromicina	150834-01	1
Euro OTC	Eritromicina	15245002	1
Euro OTC	Eritromicina	15245008	1
Euro OTC	Eritromicina	15245101	1
Euro OTC	Eritromicina	1607038	2
Euro OTC	Eritromicina	1607038/01	1
Euro OTC	Eritromicina	160703801	5
Euro OTC	Eritromicina	1607038-01	81
Euro OTC	Eritromicina	160703802	2
Euro OTC	Eritromicina	1607038-02	91
Euro OTC	Eritromicina	1607038-2	1
Euro OTC	Eritromicina	16079206	1
Euro OTC	Eritromicina	167038-01	1
Euro OTC	Eritromicina	167038-02	1
Euro OTC	Eritromicina	16G06-B03-329150	1
Euro OTC	Eritromicina	170503038-03	1
Euro OTC	Eritromicina	1705037-01	1
Euro OTC	Eritromicina	1705038	3
Euro OTC	Eritromicina	1705038_01	1
Euro OTC	Eritromicina	170503801	2
Euro OTC	Eritromicina	1705038-01	143
Euro OTC	Eritromicina	170503802	1
Euro OTC	Eritromicina	1705038-02	37
Euro OTC	Eritromicina	170503803	2
Euro OTC	Eritromicina	1705038-03	54
Euro OTC	Eritromicina	1705038-04	1
Euro OTC	Eritromicina	1705039-01	1
Euro OTC	Eritromicina	170538-03	1
Euro OTC	Eritromicina	17088005	1
Euro OTC	Eritromicina	17088203	2
Euro OTC	Eritromicina	17088204	2
Euro OTC	Eritromicina	17088210	4
Euro OTC	Eritromicina	180201E/1705038-01	1
Euro OTC	Eritromicina	181019-01	1
Euro OTC	Eritromicina	18110019-01	1
Euro OTC	Eritromicina	1811019_02	1
Euro OTC	Eritromicina	1811019-01	92
Euro OTC	Eritromicina	181101902	1
Euro OTC	Eritromicina	1811019-02	13
Euro OTC	Eritromicina	1811019-2	1
Euro OTC	Eritromicina	18111019	1
Euro OTC	Eritromicina	181119-01	1
Euro OTC	Eritromicina	19006032-01	1
Euro OTC	Eritromicina	1906032	3
Euro OTC	Eritromicina	190603201	7
Euro OTC	Eritromicina	1906032-01	106
Euro OTC	Eritromicina	1906032-02	19
Euro OTC	Eritromicina	1906032-03	3
Euro OTC	Eritromicina	190603301	1
Euro OTC	Eritromicina	190632-01	1
Euro OTC	Eritromicina	200201801	2
Euro OTC	Eritromicina	2002018-01	102
Euro OTC	Eritromicina	2002018-1	1
Euro OTC	Eritromicina	2002038-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Eritromicina	20022018-01	2
Euro OTC	Eritromicina	2007017	1
Euro OTC	Eritromicina	20070170-01	1
Euro OTC	Eritromicina	200701701	4
Euro OTC	Eritromicina	2007017-01	100
Euro OTC	Eritromicina	2007017-04	1
Euro OTC	Eritromicina	20100014-01	1
Euro OTC	Eritromicina	2010012-01	1
Euro OTC	Eritromicina	201001401	3
Euro OTC	Eritromicina	2010014-01	77
Euro OTC	Eritromicina	2010014-02	27
Euro OTC	Eritromicina	201001501	1
Euro OTC	Eritromicina	2010015-01	55
Euro OTC	Eritromicina	2010015-02	13
Euro OTC	Eritromicina	201001503	1
Euro OTC	Eritromicina	2010015-03	20
Euro OTC	Eritromicina	201004-01	1
Euro OTC	Eritromicina	21A26-F01-376732	2
Euro OTC	Eritromicina	2206001-01	23
Euro OTC	Eritromicina	220712(2010014-02)	1
Euro OTC	Eritromicina	2301053-01	5
Euro OTC	Eritromicina	2301053-02	3
Euro OTC	Eritromicina	31K190P	1
Euro OTC	Eritromicina	3613A1362	1
Euro OTC	Eritromicina	4112Q-01362	1
Euro OTC	Eritromicina	4914659	1
Euro OTC	Eritromicina	700770	1
Euro OTC	Eritromicina	80616-4	1
Euro OTC	Eritromicina	95(1705038-02	1
Euro OTC	Eritromicina	96(1811019-01)	1
Euro OTC	Eritromicina	97(1811019-02)	1
Euro OTC	Eritromicina	CEPEB022C22P	1
Euro OTC	Eritromicina	EBC/20-016	1
Euro OTC	Eritromicina	EBS/1205-M-040	1
Euro OTC	Eritromicina	EBS/1307-BM-001	1
Euro OTC	Eritromicina	EBS/1701-BM-001	4
Euro OTC	Eritromicina	EBS/18-M-003	1
Euro OTC	Eritromicina	EBS/19-022	5
Euro OTC	Eritromicina	EBS/20-016	1
Euro OTC	Eritromicina	EBS/20-040	1
Euro OTC	Eritromicina	EBS/20-041	1
Euro OTC	Eritromicina	EBS18M003	1
Euro OTC	Eritromicina	EM04022021	1
Euro OTC	Eritromicina	F02-3687508	1
Euro/ANZAG	Eritromicina	1705038-03	1
Euro/Gehe	Eritromicina	1508034-01	1
Euro/Gehe	Eritromicina	1607038-02	1
Euro/Gehe	Eritromicina	1705038-01	2
Euro/Krieger	Eritromicina	1607038-01	1
Euro/Krieger	Eritromicina	1906032-01	2
Euro/Noweda	Eritromicina	1811019-01	2
Euro/Phönix	Eritromicina	1705038-02	1
Euro/Phönix	Eritromicina	1811019-01	1
Euro/Phönix	Eritromicina	2007017-01	1
Euro/Sanacorp	Eritromicina	1607038-02	1
Euro/Sanacorp	Eritromicina	1705038-01	1
Euro	Eritromicina	1308016-02	1
euroct/gehe	Eritromicina	1308016-01	1
euroct/gehe	Eritromicina	1308016-02	2
Euroct/Gehe	Eritromicina	1409019-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Europharm/Otto	Eritromicina	1106036-05	2
EuroTOC / Noweda	Eritromicina	1409019-02	1
EurPS	Eritromicina	1409019-02	3
fagr	Eritromicina	13A02-N06	1
Fagron	Eritromicina		6
Fagron	Eritromicina	114-07-8	1
Fagron	Eritromicina	11D13-N09	2
Fagron	Eritromicina	11J06-N05	2
Fagron	Eritromicina	11J06-No5	1
Fagron	Eritromicina	1205036-01	1
Fagron	Eritromicina	12E24-N04	14
Fagron	Eritromicina	12E24-No4	1
Fagron	Eritromicina	12J30-N01	13
Fagron	Eritromicina	13175503	1
Fagron	Eritromicina	13175602	1
Fagron	Eritromicina	13175608	1
Fagron	Eritromicina	13175803	1
Fagron	Eritromicina	13175810	1
Fagron	Eritromicina	13A02N06	1
Fagron	Eritromicina	13A02-N06	9
Fagron	Eritromicina	13A02-N-06	1
Fagron	Eritromicina	13A02-N060571/680	1
Fagron	Eritromicina	13A02-No6	1
Fagron	Eritromicina	13d30-n01	1
Fagron	Eritromicina	13D30N01	1
Fagron	Eritromicina	13D30-N01	23
Fagron	Eritromicina	13D30-N01003/456	1
Fagron	Eritromicina	13D30-N010278/730	1
Fagron	Eritromicina	13D30-N010336/730	1
Fagron	Eritromicina	13f12-n21	1
Fagron	Eritromicina	13F12-N21	24
Fagron	Eritromicina	13H22-N07	7
Fagron	Eritromicina	13H22-N070126/246	1
Fagron	Eritromicina	13H22-N070228/246	1
Fagron	Eritromicina	14/30-B01	1
Fagron	Eritromicina	14/30-B01_308790	1
Fagron	Eritromicina	14/30B01300060	1
Fagron	Eritromicina	14/30-B01-300060	3
Fagron	Eritromicina	14/30B0130050	1
Fagron	Eritromicina	14/30-B01-303884	1
Fagron	Eritromicina	14/30-B01-308189	2
Fagron	Eritromicina	14/30-B01-308789	3
Fagron	Eritromicina	1409019-02	5
Fagron	Eritromicina	1430B01300059	1
Fagron	Eritromicina	1430-b01-300060	1
Fagron	Eritromicina	1430B01303884	1
Fagron	Eritromicina	1430-B01-303884	1
Fagron	Eritromicina	1430-B01-308789	1
Fagron	Eritromicina	14806-B35-290874	1
Fagron	Eritromicina	14B06-35-290873	1
Fagron	Eritromicina	14B06-B35	11
Fagron	Eritromicina	14B06-B35-290866	4
Fagron	Eritromicina	14b06-b35-290872	1
Fagron	Eritromicina	14B06-B35-290872	5
Fagron	Eritromicina	14B06-B35290873	1
Fagron	Eritromicina	14B06-B35-290873	4
Fagron	Eritromicina	14B06-B35-290874	3
Fagron	Eritromicina	14B06-B35-290875	8
Fagron	Eritromicina	14B06-B35-293508	2
Fagron	Eritromicina	14b06-b35-293509	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eritromicina	14B06-B35-293509	7
Fagron	Eritromicina	14b06b5293508	1
Fagron	Eritromicina	14F13-B02	2
Fagron	Eritromicina	14F13-B02-293487	1
Fagron	Eritromicina	14F13-B02-293488	3
Fagron	Eritromicina	14F13-B02-293490	2
Fagron	Eritromicina	14F13-B02-293511	3
Fagron	Eritromicina	14F13-B02-296464	3
Fagron	Eritromicina	14F13-B02-300061	3
Fagron	Eritromicina	14F13-B12-300061	1
Fagron	Eritromicina	14I30B01	1
Fagron	Eritromicina	14I30-B01	5
Fagron	Eritromicina	14I30-B01-3000060	1
Fagron	Eritromicina	14I30-B01-300050	2
Fagron	Eritromicina	14i30b01-300059	1
Fagron	Eritromicina	14I30-B01-300060	2
Fagron	Eritromicina	14I30-B01-300062	3
Fagron	Eritromicina	14I30-B01-300063	1
Fagron	Eritromicina	14i30-b01-303884	1
Fagron	Eritromicina	14I30-B01-303884	7
Fagron	Eritromicina	14I30-B01-306927	3
Fagron	Eritromicina	14I30-B01-308188	4
Fagron	Eritromicina	14I30B01308189	1
Fagron	Eritromicina	14I30-B01-308189	1
Fagron	Eritromicina	14I30-B01-308789	1
Fagron	Eritromicina	14i30-b01-311166	1
Fagron	Eritromicina	14I30-B01-311166	2
Fagron	Eritromicina	1508034-01	2
Fagron	Eritromicina	16/24-B10-329158	1
Fagron	Eritromicina	16/24-B10-339487	2
Fagron	Eritromicina	16/24-B10-341875	1
Fagron	Eritromicina	16/24-B10-341876	1
Fagron	Eritromicina	16079208	1
Fagron	Eritromicina	16079608	1
Fagron	Eritromicina	16G06_B03_324466	1
Fagron	Eritromicina	16G06-B03	11
Fagron	Eritromicina	16G06-B03_0003	1
Fagron	Eritromicina	16G06-B03-324462	3
Fagron	Eritromicina	16g06-b03-324463	2
Fagron	Eritromicina	16G06-B03-324463	12
Fagron	Eritromicina	16G06-B03324464	1
Fagron	Eritromicina	16G06-B03-324464	13
Fagron	Eritromicina	16G06-B03-324465	7
Fagron	Eritromicina	16G06-B03-324466	7
Fagron	Eritromicina	16G06B03-329149	1
Fagron	Eritromicina	16G06-B03-329149	4
Fagron	Eritromicina	16g06-b03-329150	1
Fagron	Eritromicina	16G06-B03-329150	6
Fagron	Eritromicina	16G06-B03-329152	2
Fagron	Eritromicina	16G06-B03-329157	6
Fagron	Eritromicina	16G06-B03-324463	1
Fagron	Eritromicina	16G08-B03	1
Fagron	Eritromicina	16J24_B10_339487	1
Fagron	Eritromicina	16j24-b10	1
Fagron	Eritromicina	16J24-B10	8
Fagron	Eritromicina	16J24-B10-329154	3
Fagron	Eritromicina	16j24-b10-329155	1
Fagron	Eritromicina	16J24-b10-329155	1
Fagron	Eritromicina	16J24-B10-329155	4
Fagron	Eritromicina	16J24-B10-329156	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eritromicina	16j24-b10-329158	1
Fagron	Eritromicina	16J24-B10-329158	3
Fagron	Eritromicina	16J24-B10-336735	7
Fagron	Eritromicina	16j24-b10-336736	1
Fagron	Eritromicina	16J24-B10-336736	4
Fagron	Eritromicina	16J24-B10-3367363	1
Fagron	Eritromicina	16J24-B10338558	1
Fagron	Eritromicina	16J24-B10-338558	1
Fagron	Eritromicina	16J24-B10-338559	1
Fagron	Eritromicina	16j24-b10-339487	1
Fagron	Eritromicina	16J24-B10-339487	9
Fagron	Eritromicina	16J24-B10-339488	3
Fagron	Eritromicina	16J24-B10-341875	7
Fagron	Eritromicina	16J24-B10-341876	1
Fagron	Eritromicina	16J24-B10-341877	1
Fagron	Eritromicina	16-j24-B10-346206	1
Fagron	Eritromicina	16J24-B10-346206	4
Fagron	Eritromicina	16J24-B10-358088	1
Fagron	Eritromicina	16J25-B10-329155	1
Fagron	Eritromicina	1705038-01	3
Fagron	Eritromicina	17088005	1
Fagron	Eritromicina	17088211	1
Fagron	Eritromicina	17088402	1
Fagron	Eritromicina	18096205	1
Fagron	Eritromicina	18096208	2
Fagron	Eritromicina	1811019-01	1
Fagron	Eritromicina	18f01-b0a-353587	1
Fagron	Eritromicina	18F05	1
Fagron	Eritromicina	18F058-B01-352501	1
Fagron	Eritromicina	18f05-b01	1
Fagron	Eritromicina	18F05-B01	7
Fagron	Eritromicina	18F-05-B01	1
Fagron	Eritromicina	18F05-B01-350897	1
Fagron	Eritromicina	18F05-B01-350906	11
Fagron	Eritromicina	18F05-B01-350907	5
Fagron	Eritromicina	18f05-b01-350908	1
Fagron	Eritromicina	18F05-B01-350908	12
Fagron	Eritromicina	18F05-B01-350909	2
Fagron	Eritromicina	18F05-B01-352500	7
Fagron	Eritromicina	18f05-b01-352501	1
Fagron	Eritromicina	18F05-B01-352501	3
Fagron	Eritromicina	18F05-B01-35358	1
Fagron	Eritromicina	18f05-b01-353586	1
Fagron	Eritromicina	18F05-B01-353586	8
Fagron	Eritromicina	18F05-B01-353587	8
Fagron	Eritromicina	18F05-B01-353588	3
Fagron	Eritromicina	18F05-B01-35387	1
Fagron	Eritromicina	18F05-B01-354817	2
Fagron	Eritromicina	18F05-B01-354818	1
Fagron	Eritromicina	18F05-B01-355773	1
Fagron	Eritromicina	18F05-B01-356076	1
Fagron	Eritromicina	18f05-b01-356705	1
Fagron	Eritromicina	18F05-B01-356705	5
Fagron	Eritromicina	18F05-B01-356706	2
Fagron	Eritromicina	18F05-B01-356707	8
Fagron	Eritromicina	18f05-b01-358087	1
Fagron	Eritromicina	18F05-B01-358087	4
Fagron	Eritromicina	18F05-B01-358088	7
Fagron	Eritromicina	18F05-B01-358362	1
Fagron	Eritromicina	18F05-B01-3586707	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eritromicina	18F05-b01-359011	1
Fagron	Eritromicina	18F05-B01-359011	1
Fagron	Eritromicina	19C21	1
Fagron	Eritromicina	19C21_B03_361400	1
Fagron	Eritromicina	19C21_B03_361402	1
Fagron	Eritromicina	19C21_B03B19	1
Fagron	Eritromicina	19c21b03	1
Fagron	Eritromicina	19C21-B03	11
Fagron	Eritromicina	19C21-B03-0003	1
Fagron	Eritromicina	19c21b03361400	1
Fagron	Eritromicina	19C21-B03-361400	13
Fagron	Eritromicina	19c21b03361401	1
Fagron	Eritromicina	19C21-B03-361401	9
Fagron	Eritromicina	19C21-B03-361402	12
Fagron	Eritromicina	19c21b03361724	1
Fagron	Eritromicina	19C21B03361724	2
Fagron	Eritromicina	19C21-B03-361724	15
Fagron	Eritromicina	19C21-B03361725	1
Fagron	Eritromicina	19C21-B03-361725	12
Fagron	Eritromicina	19C21-B03-361726	3
Fagron	Eritromicina	19C21-BO3-361726	1
Fagron	Eritromicina	19L18/F02/367780	1
Fagron	Eritromicina	19L18-F02	9
Fagron	Eritromicina	19L-18F02	1
Fagron	Eritromicina	19L18-F02-3677	1
Fagron	Eritromicina	19L18-F02-36776	1
Fagron	Eritromicina	19L18-F02-367776	1
Fagron	Eritromicina	19L18-F02-367777	9
Fagron	Eritromicina	19L18F02367778	1
Fagron	Eritromicina	19L18-F02-367778	11
Fagron	Eritromicina	19L18-F02-367779	12
Fagron	Eritromicina	19L18-F02-36778	2
Fagron	Eritromicina	19L18F02367780	1
Fagron	Eritromicina	19L18-F02-367780	2
Fagron	Eritromicina	19L18-F02-3677803	1
Fagron	Eritromicina	19L18-F02-367783	1
Fagron	Eritromicina	19L18-F02-367784	4
Fagron	Eritromicina	19L18-F02-368758	6
Fagron	Eritromicina	19L18-F02P-200319-4	1
Fagron	Eritromicina	19L18-FO2	1
Fagron	Eritromicina	19L18-FO2-367776	1
Fagron	Eritromicina	19L18-FO2-367778	1
Fagron	Eritromicina	19L18-Fo2-367779	1
Fagron	Eritromicina	19L18-FO2-367779	3
Fagron	Eritromicina	19L18-FO2-367784	2
Fagron	Eritromicina	19L18-FO2-368758	1
Fagron	Eritromicina	20/07-F06-375516	3
Fagron	Eritromicina	20107-F06	1
Fagron	Eritromicina	20107F06373880	1
Fagron	Eritromicina	20107-F06-373880	1
Fagron	Eritromicina	20107-F06375516	1
Fagron	Eritromicina	20107-F06-375516	4
Fagron	Eritromicina	20E18-F01-371571	1
Fagron	Eritromicina	20E18-F05	1
Fagron	Eritromicina	20E18-F05-371563	6
Fagron	Eritromicina	20E18-F05-371564	4
Fagron	Eritromicina	20E18-F05371565	3
Fagron	Eritromicina	20E18-F05-371565	5
Fagron	Eritromicina	20E18-F05-371566	4
Fagron	Eritromicina	20E18-F05-371567	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eritromicina	20E18-F06	9
Fagron	Eritromicina	20E18-F06-371204	1
Fagron	Eritromicina	20E18F06371570	1
Fagron	Eritromicina	20E18-F06371570	1
Fagron	Eritromicina	20E18-F06-371570	2
Fagron	Eritromicina	20E18-F06371571	1
Fagron	Eritromicina	20E18-F06-371571	7
Fagron	Eritromicina	20e18-F06-371572	1
Fagron	Eritromicina	20E18-F06-371572	2
Fagron	Eritromicina	20E18F06371573	1
Fagron	Eritromicina	20E18-F06-371573	7
Fagron	Eritromicina	20E18-F06-371573	1
Fagron	Eritromicina	20E18-F06-372103	10
Fagron	Eritromicina	20E18-F06-372104	30
Fagron	Eritromicina	20E18-F06	1
Fagron	Eritromicina	20I07-F06-373880	3
Fagron	Eritromicina	20I07-F06-3755106	1
Fagron	Eritromicina	20I07-f06-375516	1
Fagron	Eritromicina	20I07-F06-375516	8
Fagron	Eritromicina	20I07-F06-375516	1
Fagron	Eritromicina	20I17-F06-375516	1
Fagron	Eritromicina	20l07-F06-375516	1
Fagron	Eritromicina	21/13-B02	1
Fagron	Eritromicina	21/13-B02-213864	2
Fagron	Eritromicina	21/13-B02-213865	1
Fagron	Eritromicina	21/13-BO2-213864	1
Fagron	Eritromicina	21113-B02-213864	1
Fagron	Eritromicina	21113b02213865	1
Fagron	Eritromicina	21A26-F01	3
Fagron	Eritromicina	21A26-F01-37631	1
Fagron	Eritromicina	21A26-F01-376730	8
Fagron	Eritromicina	21A26-F01376731	2
Fagron	Eritromicina	21A26-F01-376731	18
Fagron	Eritromicina	21a26-f01-376732	1
Fagron	Eritromicina	21A26-F01-376732	15
Fagron	Eritromicina	21A26-F01-376734	5
Fagron	Eritromicina	21A26-Fo1-376731	2
Fagron	Eritromicina	21A26-FO1-376732	1
Fagron	Eritromicina	21F02-F02-379295	6
Fagron	Eritromicina	21I13-B02-213770	2
Fagron	Eritromicina	21I13-B02-213864	3
Fagron	Eritromicina	21I13-B02-213865	6
Fagron	Eritromicina	21l13-B02-213864	1
Fagron	Eritromicina	21l13-BO2-213864	1
Fagron	Eritromicina	21l13-BO2-213865	1
Fagron	Eritromicina	220401E	1
Fagron	Eritromicina	22102001	1
Fagron	Eritromicina	23D27-Bo1-227928	1
Fagron	Eritromicina	2OE18-F06-372104	1
Fagron	Eritromicina	3000-50	1
Fagron	Eritromicina	300059	1
Fagron	Eritromicina	31K1900P	1
Fagron	Eritromicina	3D2000P	1
Fagron	Eritromicina	4212E-01362	1
Fagron	Eritromicina	4H21P	1
Fagron	Eritromicina	510211362	1
Fagron	Eritromicina	700770-0002	1
Fagron	Eritromicina	700770-0007P-190312	1
Fagron	Eritromicina	B01-3590101	1
Fagron	Eritromicina	B02-2138604	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eritromicina	B02-213864	1
Fagron	Eritromicina	BO2-2138604	1
Fagron	Eritromicina	CEFEB001E18	1
Fagron	Eritromicina	cepb001e18	1
Fagron	Eritromicina	CEPEB001E18	2
Fagron	Eritromicina	CEPEB003D20P	4
Fagron	Eritromicina	CEPEB004H21P	2
Fagron	Eritromicina	CEPEB032B19	1
Fagron	Eritromicina	cepeb039g20p	1
Fagron	Eritromicina	CEPEB039G20P	1
Fagron	Eritromicina	CEPEB084A21	1
Fagron	Eritromicina	E-030613-1	1
Fagron	Eritromicina	E18F06-372104	1
Fagron	Eritromicina	E-250213-2	1
Fagron	Eritromicina	EB022E14	2
Fagron	Eritromicina	EB032J13	4
Fagron	Eritromicina	EB068/14	1
Fagron	Eritromicina	EB06814	1
Fagron	Eritromicina	EB078B13	1
Fagron	Eritromicina	EBS/1201-008	2
Fagron	Eritromicina	f02-3677707	1
Fagron	Eritromicina	F02-3677709	2
Fagron	Eritromicina	F02-3677803	1
Fagron	Eritromicina	F02-3677804	6
Fagron	Eritromicina	F05-3715606	1
Fagron	Eritromicina	F06-3715700	3
Fagron	Eritromicina	F06-3715703	2
Fagron	Eritromicina	F06-3721004	4
Fagron	Eritromicina	F06-3738800	1
Fagron	Eritromicina	F06-3755106	4
Fagron	Eritromicina	FO6-3715701	1
Fagron	Eritromicina	OEBA/0010516	2
Fagron	Eritromicina	OEBA/0020516	2
Fagron	Eritromicina	P-26041922/356705	1
Fargon/GEHE	Eritromicina	19C21-B03	1
Fargon/Gehe	Eritromicina	19C21-B03-361725	1
Fargon/GEHE	Eritromicina	19C21-B03-361725	1
Fargon/Noweda	Eritromicina	18F05-B01-356705	1
Fargon/Phoenix	Eritromicina	18F05-B01-358088	2
Fargon/Sanacorp	Eritromicina	16J24-B10-329158	1
Fargon	Eritromicina	19c21-b03-361725	1
Fargon	Eritromicina	20E18-F05-371566	1
Fargron / Gehe	Eritromicina	18F05-B01-350907	1
Fiebig	Eritromicina	1409019-02	1
Fiebig	Eritromicina	1607038-02	1
Fiebig	Eritromicina	1705038	1
Fiebig	Eritromicina	17088005	2
Fiebig	Eritromicina	19L18-F02-367780	1
Fiebig05.2021	Eritromicina	1607038-02	1
Finteler Apotheke	Eritromicina	1607038-02	1
Fragon/ Gehe	Eritromicina	20E18-F06-371571	1
Gatt-Koller	Eritromicina	1803029	2
GEHE 21.05.2014	Eritromicina	1308016-01	1
Gehe amax	Eritromicina	16079213	1
Gehe Rostock	Eritromicina	2007017-01	1
Gehe/ EuRho	Eritromicina	2010014-01	2
Gehe//EuRho	Eritromicina	2002018-01	1
Gehe/EuRho	Eritromicina	2002018-01	1
Gehe	Eritromicina	1106036-05	1
Gehe	Eritromicina	11D13-N09	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Eritromicina	12152105	1
Gehe	Eritromicina	12152108	1
Gehe	Eritromicina	12E24-N04	1
Gehe	Eritromicina	1308016-01	1
Gehe	Eritromicina	1308016-02	1
Gehe	Eritromicina	13189001	2
Gehe	Eritromicina	13F12-N21	1
Gehe	Eritromicina	140901901	1
Gehe	Eritromicina	1409019-01	3
Gehe	Eritromicina	1409019-02	2
Gehe	Eritromicina	15042603	1
Gehe	Eritromicina	15042611	1
Gehe	Eritromicina	15042705	1
Gehe	Eritromicina	150803401	1
Gehe	Eritromicina	1508034-01	1
Gehe	Eritromicina	15245004	1
Gehe	Eritromicina	1607038-01	2
gehe	Eritromicina	1607038-02	2
Gehe	Eritromicina	1607038-02	5
Gehe	Eritromicina	16079204	1
GEHE	Eritromicina	16079208	1
Gehe	Eritromicina	16079209	1
GEHE	Eritromicina	16079213	2
Gehe	Eritromicina	16079505	1
Gehe	Eritromicina	16079510	1
GEHE	Eritromicina	16079512	1
GEHE	Eritromicina	16079609	2
Gehe	Eritromicina	16G06-B03	1
Gehe	Eritromicina	16J24-B10-336735	1
Gehe	Eritromicina	1705038-02	1
Gehe	Eritromicina	1705038-03	1
GEHE	Eritromicina	17088008	1
Gehe	Eritromicina	17088010	1
GEHE	Eritromicina	17088203	2
Gehe	Eritromicina	17088204	1
Gehe	Eritromicina	17088210	1
Gehe	Eritromicina	18096202	1
GEHE	Eritromicina	18096210	1
Gehe	Eritromicina	180964003	1
Gehe	Eritromicina	1811019-01	1
Gehe	Eritromicina	18F05-B01-352501	1
Gehe	Eritromicina	18F05-B01-358088	1
Gehe	Eritromicina	1906032-01	1
Gehe	Eritromicina	19C21-B03-361400	1
Gehe	Eritromicina	19C21-B03-361401	1
Gehe	Eritromicina	19C21-B03-361725	2
Gehe	Eritromicina	19L18-F02-36778	1
Gehe	Eritromicina	20002259007	3
Gehe	Eritromicina	20003732002	1
Gehe	Eritromicina	20003732010	1
Gehe	Eritromicina	2002018-01	1
Gehe	Eritromicina	2007017-01	2
Gehe	Eritromicina	2010014-01	1
Gehe	Eritromicina	20E18-F06-372103	1
Gehe	Eritromicina	21A26-F01	1
GEHE	Eritromicina	21I13-B02-213865	1
Gehe	Eritromicina	22001550002	1
GEHE	Eritromicina	22001550002	1
Gehe	Eritromicina	22002200001	1
Gehe	Eritromicina	22002200003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Eritromicina	22002202003	1
GEHE	Eritromicina	2301053-01	3
Gehe	Eritromicina	2308010-01	2
Gehe	Eritromicina	3D200P	1
Gehe	Eritromicina	f02-3677707	1
Geibo	Eritromicina	20002259003	1
Geilenkirchen	Eritromicina	16J24B10-339488	1
Geilenkirchen	Eritromicina	17088210	2
Geilenkirchen	Eritromicina	17088309	1
Geilenkirchen	Eritromicina	18096205	1
Geilenkirchen	Eritromicina	19L18-F02-367780	1
gepepharm GmbH	Eritromicina	13175502	1
GUMO	Eritromicina	19C21-B03-361725	1
GUMO	Eritromicina	19L18-F02-3677708	1
GUMO	Eritromicina	19L18-F02-3687508	1
GUMO	Eritromicina	20E18-F06	1
GUMO	Eritromicina	F02-3677708	1
Gutenberg-Apotheke	Eritromicina	13175608	1
Hedinger	Eritromicina	15245002	2
Ichthyol-Gesellschaft	Eritromicina	161020E/1607038-01	1
Jenapharm/Phönix	Eritromicina	1607036-01	1
JENNE	Eritromicina	18096202	2
Jenne	Eritromicina	20003732007	1
Kehr	Eritromicina	1705038-01	1
Kehr	Eritromicina	21002041010	1
Kehr	Eritromicina	22002200004	2
Kehr	Eritromicina	226001-01	1
Kehr	Eritromicina	2301053-01	1
Klenk	Eritromicina	EB068I14	1
Klosterring	Eritromicina	CEPEB001E18	1
Krieger	Eritromicina	16G06-B03-329150	1
Krieger	Eritromicina	16J24-B10-336735	1
Krieger	Eritromicina	16J24-B10-341876	1
Krieger	Eritromicina	3402	1
L12	Eritromicina	18096203	1
L30	Eritromicina	17088208	1
Lamotte	Eritromicina	18096406	1
Midas	Eritromicina	16079609	1
Mikrobiell	Eritromicina	1705038-01	1
Mömerzheim	Eritromicina	17088001	1
Nachprüfung	Eritromicina	13175810	1
Noweda 23.08.2019	Eritromicina	1811019-01	1
Noweda Taucha	Eritromicina	21002041001	1
Noweda/Euro	Eritromicina	1607038-01	2
Noweda/Fragron	Eritromicina	18F05-B01-359011	1
Noweda/Gehe	Eritromicina	14B06-B35-293508	1
Noweda	Eritromicina	11195411	2
Noweda	Eritromicina	11195413	1
Noweda	Eritromicina	12152108	2
Noweda	Eritromicina	12152201	1
Noweda	Eritromicina	12E24-N04	1
Noweda	Eritromicina	130801602	2
Noweda	Eritromicina	13175603	2
Noweda	Eritromicina	13175608	1
Noweda	Eritromicina	14044006	1
Noweda	Eritromicina	14044114	1
Noweda	Eritromicina	150803401	1
Noweda	Eritromicina	15245101	1
Noweda	Eritromicina	160703801	1
Noweda	Eritromicina	1607038-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Eritromicina	16079502	1
Noweda	Eritromicina	16079606	1
Noweda	Eritromicina	16J24-B10	1
Noweda	Eritromicina	16J24-B10-329156	1
Noweda	Eritromicina	1705038-02	2
Noweda	Eritromicina	17088001	1
Noweda	Eritromicina	17088003	1
Noweda	Eritromicina	17088004	1
Noweda	Eritromicina	17088013	1
Noweda	Eritromicina	17088208	1
Noweda	Eritromicina	17088404	1
Noweda	Eritromicina	17088405	2
Noweda	Eritromicina	18096201	1
Noweda	Eritromicina	18096203	1
Noweda	Eritromicina	18096302	1
Noweda	Eritromicina	180964001	1
Noweda	Eritromicina	1811019-01	1
Noweda	Eritromicina	1906032-01	3
Noweda	Eritromicina	19C21-B03-361400	1
Noweda	Eritromicina	20002259004	1
Noweda	Eritromicina	20002259006	1
Noweda	Eritromicina	20003731001	2
Noweda	Eritromicina	20003731003	1
Noweda	Eritromicina	20003731004	1
Noweda	Eritromicina	20003731005	1
Noweda	Eritromicina	2010014-01	1
Noweda	Eritromicina	20I07-F06-375516	1
Noweda	Eritromicina	21002041004	7
Noweda	Eritromicina	220022000002	1
Noweda	Eritromicina	2206001-01	3
Noweda	Eritromicina	23D27-B01-227929	1
NOWEDA	Eritromicina	23D27-B01-227929	2
Noweda	Eritromicina	24C25-B34-001113	2
Noweda	Eritromicina	P2019/92	1
Noweda12/2025	Eritromicina	22002200002	1
Noweda21.04.2015	Eritromicina	14044110	1
OTG/Gehe	Eritromicina	1409019-01	1
Otto Fischar	Eritromicina	16G06-B03-329150	1
Parthe Apotheke	Eritromicina	147/19	1
Parthe Apotheke	Eritromicina	56/21	1
ph.Eur	Eritromicina	2301053-01	1
Ph.Euro/Noweda	Eritromicina	2010015-01	1
Phagron	Eritromicina		1
PHOENIX 08.05.2014	Eritromicina	13175604	1
PHOENIX 08.05.2014	Eritromicina	13175608	2
Phoenix 10.02.2020	Eritromicina	1906032-01	1
Phoenix 28.11.2018	Eritromicina	17088004	1
Phoenix/Cealo	Eritromicina	17088004/0918E-01362	1
Phoenix	Eritromicina	12152201	2
Phoenix	Eritromicina	13175608	1
Phoenix	Eritromicina	14044106	1
Phoenix	Eritromicina	15042609	1
Phoenix	Eritromicina	15042811	1
Phoenix	Eritromicina	16079501	1
Phoenix	Eritromicina	1705038-01	1
Phoenix	Eritromicina	17088403	1
Phoenix	Eritromicina	18096205	1
Phoenix	Eritromicina	18096302	1
Phoenix	Eritromicina	180964003	1
Phoenix	Eritromicina	18096401	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Eritromicina	1906032-01	2
PHOENIX	Eritromicina	19C21-B03	1
Phoenix	Eritromicina	20003731001	1
Phoenix	Eritromicina	20003731004	4
Phoenix	Eritromicina	2002018-01	1
Phoenix	Eritromicina	2007017-01	1
Phoenix	Eritromicina	201001501	1
Phoenix	Eritromicina	21002041014	1
Phoenix	Eritromicina	22002200004	1
Phoenix	Eritromicina	22002203001	1
Phoenix	Eritromicina	23003387001	2
Phoenix	Eritromicina	3104	1
Phoenix	Eritromicina	3207	1
Phönix WE: 23.09.17...	Eritromicina	16079604	1
Phönix Eurho	Eritromicina	2002018-01	1
Phönix Gotha	Eritromicina	18096303	1
Phönix Gotha	Eritromicina	18096403	1
Phönix WE:30.07.2016...	Eritromicina	15245101	1
Phönix	Eritromicina	1205036-02	1
Phönix	Eritromicina	121427016	1
Phönix	Eritromicina	14044201	1
Phönix	Eritromicina	14B06-B35	1
Phönix	Eritromicina	14F13-B02-293511	1
phönix	Eritromicina	15042611	1
phönix	Eritromicina	15042813	1
Phönix	Eritromicina	15042813	2
phönix	Eritromicina	15245101	1
phönix	Eritromicina	16079203	1
Phönix	Eritromicina	16079205	1
Phönix	Eritromicina	16079210	1
Phönix	Eritromicina	1705038-01	3
Phönix	Eritromicina	1705038-03	1
Phönix	Eritromicina	17088002	1
Phonix	Eritromicina	17088005	1
Phönix	Eritromicina	17088301	1
Phönix	Eritromicina	17088306	1
Phönix	Eritromicina	17088404	1
Phönix	Eritromicina	18096209	1
Phönix	Eritromicina	1811019-01	3
PHÖNIX	Eritromicina	1906032	1
Phönix	Eritromicina	1906032-01	4
Phönix	Eritromicina	19C21-B03-361724	2
Phönix	Eritromicina	19118-F02-367779	1
Phönix	Eritromicina	200202018-01	1
Phönix	Eritromicina	200952209	1
Phönix	Eritromicina	2010014-01	1
PHÖNIX	Eritromicina	2010014-01	1
Phönix	Eritromicina	2010015-01	1
Phönix	Eritromicina	20E18-F06-372103	1
Phönix	Eritromicina	21002041009	1
Phönix	Eritromicina	21002041010	1
Phönix	Eritromicina	22001550002	1
Phönix	Eritromicina	22002199001	1
Phönix	Eritromicina	22002200002	2
Phönix	Eritromicina	22002200004	4
Phönix	Eritromicina	22002200005	1
Phönix	Eritromicina	23D27-B01-227928	1
Rondell Apotheke	Eritromicina	15042803	1
Röntgen	Eritromicina	1811019-01	4
Röntgen	Eritromicina	2002018-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Röntgen	Eritromicina	2007017-01	1
Sanacopr	Eritromicina		1
Sanacorp/apo-ident	Eritromicina	1705038-03	1
Sanacorp/EuRho	Eritromicina	17088306	1
Sanacorp	Eritromicina		1
Sanacorp	Eritromicina	1106036-04	1
Sanacorp	Eritromicina	1205035-02	1
Sanacorp	Eritromicina	12152202	1
Sanacorp	Eritromicina	12156208	1
Sanacorp	Eritromicina	1308016-01	1
Sanacorp	Eritromicina	1308016-02	1
Sanacorp	Eritromicina	13H22-N07	1
Sanacorp	Eritromicina	1409019-01	1
Sanacorp	Eritromicina	16079612	1
Sanacorp	Eritromicina	16J24-B10	2
Sanacorp	Eritromicina	16J24B10-338559	1
Sanacorp	Eritromicina	16J24-B10-338559	1
Sanacorp	Eritromicina	1705038-03	1
Sanacorp	Eritromicina	17088002	1
Sanacorp	Eritromicina	17088010	1
Sanacorp	Eritromicina	170880403	1
Sanacorp	Eritromicina	17088203	2
Sanacorp	Eritromicina	17088302	1
Sanacorp	Eritromicina	17088402	1
Sanacorp	Eritromicina	17088404	1
Sanacorp	Eritromicina	18096204	1
Sanacorp	Eritromicina	18096210	1
Sanacorp	Eritromicina	18096404	1
Sanacorp	Eritromicina	18096405	1
sanacorp	Eritromicina	18096406	1
Sanacorp	Eritromicina	181101901	1
Sanacorp	Eritromicina	18F05-B01-350908	2
sanacorp	Eritromicina	1906032-01	1
Sanacorp	Eritromicina	1906032-01	1
Sanacorp	Eritromicina	19C21-B03	1
Sanacorp	Eritromicina	19C21-B03-361401	1
Sanacorp	Eritromicina	19C21-B03-361725	1
Sanacorp	Eritromicina	19L18-F02-368758	1
Sanacorp	Eritromicina	20071017-01	1
Sanacorp	Eritromicina	20100114-01	1
Sanacorp	Eritromicina	2010014-02	1
Sanacorp	Eritromicina	20E18-F06-3721004	1
Sanacorp	Eritromicina	20E18-F06-372104	1
Sanacorp	Eritromicina	21002041004	1
Sanacorp	Eritromicina	21002041014	1
Sanacorp	Eritromicina	21002046001	1
Sanacorp	Eritromicina	21f02-f02-379295	1
Sanacorp	Eritromicina	21I13-B02-213865	1
Sanacorp	Eritromicina	22001550005	2
Sanacorp	Eritromicina	2206001-01	1
Sanacorp	Eritromicina	2301053-01	1
Sanacorp	Eritromicina	23H23-B04-231446	2
Sanacorp	Eritromicina	23H23-B04-236846	1
Sanacorp	Eritromicina	31K190P	1
Sanacorp	Eritromicina	59/AKD51	1
Sanacorp	Eritromicina	60/AKD52	1
Sanacorp;19.03.15;30,50EUR	Eritromicina	1409019-01	1
Sm Biomed / Gehe	Eritromicina	15245002	1
Sm Biomed / Gehe	Eritromicina	16079202	1
Sm Biomed / Gehe	Eritromicina	17088013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
SM Biomed Sdn Bhd/Phoenix	Eritromicina	2010015-01	1
SM Biomed Sdn. Bhd	Eritromicina	20020018-01	1
SM Biomed Sdn	Eritromicina	18096405	1
SM Biomed/Noweda	Eritromicina	EBD/20-003	1
SM Biomed/Phoenix	Eritromicina	EBD/18-003	2
Spangro	Eritromicina	16079205	1
Spangro	Eritromicina	16G06-B-03-329151	1
Spangro_21.05.2019	Eritromicina	1705038-03	1
Unisan	Eritromicina	140901902	1
VDL	Eritromicina	11195407	1
VDL	Eritromicina	160703801	1
wepa	Eritromicina	2206001-01	1
Wolff/AHD	Eritromicina	15245004	1

- 229 747 spectra from 1515 *Apo-Ident* customers from a total of 48 315 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Eritromicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Eritromicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	840	0	201 244
Type C	0	6167	153	229 747

The substance/substance group *Eritromicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2857 %)
Type C	100.0000 % (> 99.9007 %)	97.5791 % (> 97.5316 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21056	21890	11,02	120,94
21323	22438	6,06	121,76
21651	21651	0,00	137,31
21669	21651	14,77	127,63
21890	21890	0,00	123,28
22438	22438	0,00	123,28
22832	22832	0,00	120,52
23438	23438	0,00	120,22
24420	24420	0,00	138,35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Escina, hidrossolúvel**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20377-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Escina, hidrossolúvel; Aescinum solubile

Special notes

When selecting the *Escina, hidrossolúvel* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Escina, hidrossolúvel	7	3	3

Second-stage model

For differentiation of the substance/substance group *Escina, hidrossolúvel* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Escina, hidrossolúvel* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	48,99	–
Fosfato sódico de riboflavina hidratado	76,07	–
⋮	⋮	⋮
Furoato de mometasona	>50	68,48
Citrato monobásico de magnésio, hid…	>50	86,49
Hidrocortisona	>50	94,33
Sulfato de atropina	>50	120,90
Quinolina amarela	>50	177,01
Sorbato de potássio	>50	263,24
Sacarina sódica	>50	263,65
Orotato de cálcio di-hidratado	>50	387,40
Cloridrato de propranolol	>50	562,70
Fenitoína	>50	906,19

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Escina, hidrossolúvel* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Escina, hidrossolúvel*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Escina, hidrossolúvel	1310020-01	21238	40	AR-15-FG-005777-01
Euro OTC	Escina, hidrossolúvel	1506038	21838	60	20150708*
Euro OTC	Escina, hidrossolúvel	1605021	22684	40	20160609*
Euro OTC	Escina, hidrossolúvel	2009019	25410	40	20201009*
Euro OTC	Escina, hidrossolúvel	2106010	25707	50	20210715*
Fagron	Escina, hidrossolúvel	12K22-N13	21237	40	20121127
Fagron	Escina, hidrossolúvel	12I07-B40-306607	22610	40	1610369

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 310 spectra of 7 reference samples from the substance/substance group *Escina, hidrossolúvel*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 652 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Escina, hidrossolúvel*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Escina, hidrossolúvel	1612012	22988	40
Euro OTC	Escina, hidrossolúvel	1807015-01	24187	40
Euro OTC	Escina, hidrossolúvel	1911023	24939	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Escina, hidrossolúvel*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Escina, hidrossolúvel	1108038	1
Euro OTC	Escina, hidrossolúvel	1310020-01	1
Euro OTC	Escina, hidrossolúvel	1612012-01	3
Fagron	Escina, hidrossolúvel	30691/M3	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Escina, hidrossolúvel* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Escina, hidrossolúvel* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	120	0	201 964
Type C	0	6	0	236 061

The substance/substance group *Escina, hidrossolúvel* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21237	21238	6,88	112,11
21238	21238	0,00	106,44
21838	21838	0,00	126,94
22610	22610	0,00	115,65
22684	22684	0,00	121,82
25410	25410	0,00	117,02
25707	25707	0,00	127,23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Espironolactona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21032-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Espironolactona

Special notes

When selecting the *Espironolactona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Espironolactona	9	15	231

Second-stage model

For differentiation of the substance/substance group *Espironolactona* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Espironolactona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	104,86	–
⋮	⋮	⋮
Progesterona	>50	62,85
Propionato de testosterona	>50	66,04
Iodopovidona	>50	76,66
Ácido fusídico	>50	92,10
Ubidecarenona	>50	136,83
Povidona	>50	151,96

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Espironolactona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Espironolactona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Espironolactona	14378715	22385	40	20150211
Caelo	Espironolactona	160773	22444	60	20160415*
Caelo	Espironolactona	190158	24548	40	20190308*
Caelo	Espironolactona	20001838	25213	40	20200617*
Euro OTC	Espironolactona	1212034-01	21032	50	1403151
Euro OTC	Espironolactona	1212034-01	21076	42	20130215
Euro OTC	Espironolactona	1602006	22369	45	20160309*
Euro OTC	Espironolactona	2006012	25311	40	20200821*
Euro OTC	Espironolactona	2006012	25311SI	33	20200821*
Fagron	Espironolactona	15G22-B10-311159	22386	40	20150728
Fagron	Espironolactona	16E20-B06-322016	22942	40	20160531

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 470 spectra of 11 reference samples from the substance/substance group *Espironolactona*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 492 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 736 spectra of 21 reference samples from the substance/substance group *Espironolactona*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Espironolactona	16077305	22954	40
Caelo	Espironolactona	171165	23327	40
Caelo	Espironolactona	172432	23660	40
Caelo	Espironolactona	182080	24391	40
Caelo	Espironolactona	191979	24748	40
Caelo	Espironolactona	22000904013	26739	40
Euro OTC	Espironolactona	1612002	22909	40
Euro OTC	Espironolactona	1711013	23888	40
Euro OTC	Espironolactona	1809020	24324	40
Euro OTC	Espironolactona	1907001	24782	40
Euro OTC	Espironolactona	2203010	26086	40
Fagron	Espironolactona	22B07-B14-227278	26543	40
Fagron	Espironolactona	120A20240801	BR20035	40
Fagron	Espironolactona	120A20240802	BR20036	40
Fagron	Espironolactona	10A20240801	BR20037SI	20
Caelo	Espironolactona	22000904013	26739SI	31
Euro OTC	Espironolactona	2203010	26086SI	10
Fagron	Espironolactona	22B07-B14-227278	26543SI	35
Fagron	Espironolactona	120A20240801	BR20035SI	20
Fagron	Espironolactona	120A20240802	BR20036SI	20
Fagron	Espironolactona	120A20240801	BR20037	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 348 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1279 spectra from 468 *Apo-Ident* customers from 241 batches from the substance/substance group *Espironolactona*.

- Among them are spectra of independent samples from 231 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Espironolactona		1
	Espironolactona	22000904001	2
	Espironolactona	22000904002	1
	Espironolactona	22000904007	2
	Espironolactona	22000904008	6
	Espironolactona	22000904011	1
	Espironolactona	22000904012	5
	Espironolactona	22000904013	7
	Espironolactona	22000904015	12
	Espironolactona	22000904018	2
	Espironolactona	23001294004	1
	Espironolactona	23001294005	8
	Espironolactona	23001294006	2
	Espironolactona	24000134003	1
AHD 23.07.2020	Espironolactona	190158003	1
AHD	Espironolactona	22000904008	1
AHD	Espironolactona	22000904012	1
AHD	Espironolactona	23001294005	1
AHD	Espironolactona	24000134003	1
Alliance Healthcare	Espironolactona	12049119	1
Alliance Healthcare	Espironolactona	12049129	1
Alliance	Espironolactona	22000904018	1
Alliance	Espironolactona	24000134003	1
Anzag	Espironolactona	191163002	2
Anzag	Espironolactona	20003886003	2
Anzag	Espironolactona	21000085007	1
apomix	Espironolactona	16077320	1
Caelo	Espironolactona		1
Caelo	Espironolactona	10159914	1
Caelo	Espironolactona	1090216	1
Caelo	Espironolactona	10H24-N10	1
Caelo	Espironolactona	11042602	1
Caelo	Espironolactona	11042607	1
Caelo	Espironolactona	1110917/16077320	1
Caelo	Espironolactona	11G28-N03	1
Caelo	Espironolactona	12049103	1
Caelo	Espironolactona	12049105	2
Caelo	Espironolactona	12049109	1
Caelo	Espironolactona	12049110	2
Caelo	Espironolactona	12049118	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Espironolactona	12049123	3
Caelo	Espironolactona	12049130	4
Caelo	Espironolactona	13124303	7
Caelo	Espironolactona	13124304	7
Caelo	Espironolactona	13124309	6
Caelo	Espironolactona	13124314	2
Caelo	Espironolactona	13124315	6
Caelo	Espironolactona	13124317	3
Caelo	Espironolactona	13124320	3
Caelo	Espironolactona	13124321	2
Caelo	Espironolactona	131243315	1
Caelo	Espironolactona	1314309	1
Caelo	Espironolactona	13190309	3
Caelo	Espironolactona	140202901	1
Caelo	Espironolactona	1437807	1
Caelo	Espironolactona	1437815	1
Caelo	Espironolactona	14378701	2
Caelo	Espironolactona	14378702	4
Caelo	Espironolactona	14378703	1
Caelo	Espironolactona	14378709	4
Caelo	Espironolactona	14378710	5
Caelo	Espironolactona	14378715	8
Caelo	Espironolactona	14378717	3
Caelo	Espironolactona	14378718	9
Caelo	Espironolactona	14378719	1
Caelo	Espironolactona	14378721	2
Caelo	Espironolactona	1438721	1
Caelo	Espironolactona	1496810000858	1
Caelo	Espironolactona	150401601	1
Caelo	Espironolactona	15G22-B10	1
Caelo	Espironolactona	160773	1
Caelo	Espironolactona	16077302	16
Caelo	Espironolactona	16077303	17
Caelo	Espironolactona	16077305	10
Caelo	Espironolactona	16077306	8
Caelo	Espironolactona	16077307	1
Caelo	Espironolactona	16077309	7
Caelo	Espironolactona	1607731	1
Caelo	Espironolactona	16077311	14
Caelo	Espironolactona	16077312	20
Caelo	Espironolactona	16077312/1230817	1
Caelo	Espironolactona	16077316	1
Caelo	Espironolactona	16077319	5
Caelo	Espironolactona	16077320	11
Caelo	Espironolactona	16077324	1
Caelo	Espironolactona	16077325	20
Caelo	Espironolactona	16077326	17
Caelo	Espironolactona	161200201	1
Caelo	Espironolactona	16A14-B05-317123	1
Caelo	Espironolactona	16D15-B06-320903	1
Caelo	Espironolactona	16H20-B06-322016	1
Caelo	Espironolactona	17116501	1
Caelo	Espironolactona	171165012	1
Caelo	Espironolactona	17116502	9
Caelo	Espironolactona	17H16-B05-341740	1
Caelo	Espironolactona	17H16-B05-344771	1
Caelo	Espironolactona	18004803	12
Caelo	Espironolactona	18004902	3
Caelo	Espironolactona	18004904	20
Caelo	Espironolactona	18004908	12

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Espironolactona	18004912	1
Caelo	Espironolactona	18004913	4
Caelo	Espironolactona	18004915	13
Caelo	Espironolactona	18004915P-190531-5	1
Caelo	Espironolactona	18004917	22
Caelo	Espironolactona	18004917P-190604-1	1
Caelo	Espironolactona	18004919	1
Caelo	Espironolactona	18004920	17
Caelo	Espironolactona	18004922	1
Caelo	Espironolactona	180208003	1
Caelo	Espironolactona	18205004	1
Caelo	Espironolactona	18208003	12
Caelo	Espironolactona	18208004	11
Caelo	Espironolactona	18208005	1
Caelo	Espironolactona	18208008	15
Caelo	Espironolactona	18208008P-191007-1	1
Caelo	Espironolactona	18208010	12
Caelo	Espironolactona	18A24-B03-348018	5
Caelo	Espironolactona	190158001	15
Caelo	Espironolactona	190158003	1
Caelo	Espironolactona	190158004	1
Caelo	Espironolactona	19015801	1
Caelo	Espironolactona	19015802	1
Caelo	Espironolactona	190158022	1
Caelo	Espironolactona	19015803	23
Caelo	Espironolactona	19015804	16
Caelo	Espironolactona	19015805	3
Caelo	Espironolactona	19015809	8
Caelo	Espironolactona	19015809P-200507-2	1
Caelo	Espironolactona	1907001-01	2
Caelo	Espironolactona	191163001	9
Caelo	Espironolactona	191163002	27
Caelo	Espironolactona	191163003	1
Caelo	Espironolactona	191163004	8
Caelo	Espironolactona	191163008	13
Caelo	Espironolactona	20003605013	1
Caelo	Espironolactona	2000386003	1
Caelo	Espironolactona	20003886003	30
Caelo	Espironolactona	20003886004	2
Caelo	Espironolactona	20003886005	8
Caelo	Espironolactona	2013U-03249	1
Caelo	Espironolactona	210000085007	1
Caelo	Espironolactona	21000085001	2
Caelo	Espironolactona	21000085002	15
Caelo	Espironolactona	210000850022	1
Caelo	Espironolactona	21000085004	12
Caelo	Espironolactona	21000085006	1
Caelo	Espironolactona	21000085007	12
Caelo	Espironolactona	21000085008	6
Caelo	Espironolactona	21000085009	20
Caelo	Espironolactona	21000085010	11
Caelo	Espironolactona	21000085012	2
Caelo	Espironolactona	21000085015	11
Caelo	Espironolactona	21000085017	11
Caelo	Espironolactona	21000085018	3
Caelo	Espironolactona	2100008508	1
Caelo	Espironolactona	2100008509	2
Caelo	Espironolactona	210000855007	1
Caelo	Espironolactona	2100085007	1
Caelo	Espironolactona	2100085017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Espironolactona	22000904001	12
Caelo	Espironolactona	22000904002	14
Caelo	Espironolactona	22000904008	2
Caelo	Espironolactona	22000904012	2
Caelo	Espironolactona	2200090404002	1
Caelo	Espironolactona	22121701	1
Caelo	Espironolactona	5013Q-03249	1
Caeol/Noweda	Espironolactona	16077303	1
Caeol/Noweda	Espironolactona	16077305	2
Caeol/Noweda	Espironolactona	18208008	1
Caesar & Loretz GmbH…	Espironolactona	18004915	1
Caesar & Loretz GmbH…	Espironolactona	18004920	1
Caesar & Loretz GmbH…	Espironolactona	190158001	3
Caesar & Loretz GmbH…	Espironolactona	22000904002	1
Caesar & Loretz GmbH…	Espironolactona	21000085010	1
Caesar & Loretz GmbH…	Espironolactona	22000904001	1
Caesar & Loretz GmbH…	Espironolactona	19015803	1
Caesar & Loretz GmbH/AHD	Espironolactona	21000085002	1
Caesar & Loretz GmbH/AHD	Espironolactona	21000085010	2
Caesar & Loretz GmbH…	Espironolactona	191163008	1
Caesar & Loretz GmbH/Gehe	Espironolactona	190158001	2
Caesar & Loretz GmbH/Gehe	Espironolactona	19015803	2
Caesar & Loretz GmbH/Gehe	Espironolactona	19015804	1
Caesar & Loretz GmbH/Gehe	Espironolactona	191163004	1
Caesar & Loretz GmbH/GEHE	Espironolactona	191163008	1
Caesar & Loretz GmbH/GEHE	Espironolactona	21000085002	1
Caesar & Loretz GmbH/Gehe	Espironolactona	21000085007	1
Caesar & Loretz GmbH/Kehr	Espironolactona	22000904001	2
Caesar & Loretz GmbH…	Espironolactona	18208010	5
Caesar & Loretz GmbH…	Espironolactona	19015804	1
Caesar & Loretz GmbH…	Espironolactona	19015809	1
Caesar & Loretz GmbH…	Espironolactona	191163004	1
Caesar & Loretz GmbH…	Espironolactona	21000085007	1
Caesar & Loretz GmbH…	Espironolactona	18208010	1
Caesar & Loretz GmbH…	Espironolactona	190158004	1
Caesar & Loretz GmbH…	Espironolactona	19015803	2
Caesar & Loretz GmbH…	Espironolactona	20003886003	1
Caesar & Loretz GmbH…	Espironolactona	21000085004	1
Caesar & Loretz GmbH…	Espironolactona	18004915	1
Caesar & Loretz GmbH	Espironolactona	12049129	1
Caesar & Loretz GmbH	Espironolactona	18004917	1
Caesar & Loretz GmbH	Espironolactona	18004920	2
Caesar & Loretz GmbH	Espironolactona	18208003	4
Caesar & Loretz GmbH	Espironolactona	18208004	1
Caesar & Loretz GmbH	Espironolactona	18208008	4
Caesar & Loretz GmbH	Espironolactona	18208010	3
Caesar & Loretz GmbH	Espironolactona	190158001	7
Caesar & Loretz GmbH	Espironolactona	190158004	2
Caesar & Loretz GmbH	Espironolactona	19015803	2
Caesar & Loretz GmbH	Espironolactona	19015804	11
Caesar & Loretz GmbH	Espironolactona	19015809	3
Caesar & Loretz GmbH	Espironolactona	191163001	2
Caesar & Loretz GmbH	Espironolactona	191163002	7
Caesar & Loretz GmbH	Espironolactona	191163004	3
Caesar & Loretz GmbH	Espironolactona	191163008	6
Caesar & Loretz GmbH	Espironolactona	20003886002	1
Caesar & Loretz GmbH	Espironolactona	20003886003	4
Caesar & Loretz GmbH	Espironolactona	20003886004	1
Caesar & Loretz GmbH	Espironolactona	20003886005	8
Caesar & Loretz GmbH	Espironolactona	21000085001	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Espironolactona	21000085002	5
Caesar & Loretz GmbH	Espironolactona	21000085004	7
Caesar & Loretz GmbH	Espironolactona	21000085006	2
Caesar & Loretz GmbH	Espironolactona	21000085007	7
Caesar & Loretz GmbH	Espironolactona	21000085008	6
Caesar & Loretz GmbH	Espironolactona	21000085009	4
Caesar & Loretz GmbH	Espironolactona	21000085010	10
Caesar & Loretz GmbH	Espironolactona	21000085015	6
Caesar & Loretz GmbH	Espironolactona	21000085017	7
Caesar & Loretz GmbH	Espironolactona	21000085018	2
Caesar & Loretz GmbH	Espironolactona	22000904001	10
Caesar & Loretz GmbH	Espironolactona	22000904002	3
Caesar & Loretz GmbH	Espironolactona	22000904004	1
Caesar & Loretz GmbH	Espironolactona	22000904008	1
Caesar & Loretz GmbH	Espironolactona	22000904018	1
Caesar & Loretz GmbH…	Espironolactona	20003886005	1
Caesar u Loretz	Espironolactona	12049119	1
Caesar u. Loretz / G…	Espironolactona	18208010	1
Caesar und Loretz GmbH	Espironolactona	191163008	1
Caesar&Loretz GmbH	Espironolactona	19015804	1
Caesar&loretz,Anzag	Espironolactona	13124309	1
Caesar&loretz,Phoenix	Espironolactona	11042603	1
Caesar&loretz,Phoenix	Espironolactona	11042613	1
Caesar/Lorenz	Espironolactona	13124303	1
Cealo/Gehe	Espironolactona	18004904	2
EuRho / Noweda	Espironolactona	200612-01	1
Eurho/Anzag	Espironolactona	190700101	1
EuRho	Espironolactona	1101013-01	1
Euro OTC	Espironolactona	1000403502	1
Euro OTC	Espironolactona	1004035	1
Euro OTC	Espironolactona	1101013-01	1
Euro OTC	Espironolactona	1212034-01	6
Euro OTC	Espironolactona	1402029-01	1
Euro OTC	Espironolactona	14378721	1
Euro OTC	Espironolactona	1504016-01	3
Euro OTC	Espironolactona	16020006-01	1
Euro OTC	Espironolactona	1602006-01	5
Euro OTC	Espironolactona	1602006-02	1
Euro OTC	Espironolactona	1612002_01	1
Euro OTC	Espironolactona	161200201	1
Euro OTC	Espironolactona	1612002-01	5
Euro OTC	Espironolactona	16E20-B06-322016	1
Euro OTC	Espironolactona	171101301	1
Euro OTC	Espironolactona	1711013-01	12
Euro OTC	Espironolactona	180902001	1
Euro OTC	Espironolactona	1809020-01	5
Euro OTC	Espironolactona	1809020-02	1
Euro OTC	Espironolactona	190700-01	1
Euro OTC	Espironolactona	1907001-01	9
Euro OTC	Espironolactona	2006012-01	5
Euro OTC	Espironolactona	3513E-03249	1
Fagron	Espironolactona		1
Fagron	Espironolactona	10C29-N09	1
Fagron	Espironolactona	10H24-N10	1
Fagron	Espironolactona	12/17-n01	1
Fagron	Espironolactona	12/17-N01	1
Fagron	Espironolactona	12I17-N01	1
Fagron	Espironolactona	12J15-N04	1
Fagron	Espironolactona	13D12-N08	2
Fagron	Espironolactona	13G03-N09	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Espironolactona	13G16-B08	1
Fagron	Espironolactona	13G16-B08-288051	1
Fagron	Espironolactona	14B20B06294618	1
Fagron	Espironolactona	14B20-B06-294618	5
Fagron	Espironolactona	14j02-b02-303621	1
Fagron	Espironolactona	14J02-B02-303621	5
Fagron	Espironolactona	14J02-B02-303622	1
Fagron	Espironolactona	14J02-B303621	1
Fagron	Espironolactona	15G22-B10-311159	2
Fagron	Espironolactona	16A14-B05	1
Fagron	Espironolactona	16A14-B05-317123	1
Fagron	Espironolactona	16A14-B05-525187	1
Fagron	Espironolactona	16D15-B06-320903	1
Fagron	Espironolactona	16E20-B06-322016	1
Fagron	Espironolactona	16E20-B06-325478	2
Fagron	Espironolactona	16I06-B04	1
Fagron	Espironolactona	16I06B04329443	1
Fagron	Espironolactona	16I06-B04-329443	1
Fagron	Espironolactona	17116502	1
Fagron	Espironolactona	17E22-B11-335454	2
Fagron	Espironolactona	17E22-B11-335455	2
Fagron	Espironolactona	17H16-B05	2
Fagron	Espironolactona	17H16-B05-341739	2
Fagron	Espironolactona	17H16-B05-344771	3
Fagron	Espironolactona	18208003	1
Fagron	Espironolactona	18A24-B03	1
Fagron	Espironolactona	18A24-B03-349548	6
Fagron	Espironolactona	18A24-B03-354314	2
Fagron	Espironolactona	18G12-B01-356145	3
Fagron	Espironolactona	19C29-B06-191465	3
Fagron	Espironolactona	19H23-B06-194244	1
Fagron	Espironolactona	19H23-B06-194245	1
Fagron	Espironolactona	19H23-B06-194567	1
Fagron	Espironolactona	19H23-B06-194569	2
Fagron	Espironolactona	19H23-BO6-194245	1
Fagron	Espironolactona	2006012-01	2
Fagron	Espironolactona	20B24-B04	2
Fagron	Espironolactona	20B24-B04-200519	1
Fagron	Espironolactona	20B24-B04-200520	5
Fagron	Espironolactona	20H19-B01-202267	2
Fagron	Espironolactona	20H19-B01-213618	2
Fagron	Espironolactona	21H27-B05-217974	3
Fagron	Espironolactona	21H27-B05-222385	1
Fagron	Espironolactona	2415E-03249	1
Fagron	Espironolactona	2517Q03249	1
Fagron	Espironolactona	2918E-03249	1
Fagron	Espironolactona	80616-7	1
Fagron	Espironolactona	B01-2022607	1
Fagron	Espironolactona	B04-2005109	1
Fagron	Espironolactona	B04-2005200	1
Fagron	Espironolactona	eln170404	1
Fagron	Espironolactona	SA1063	2
Fiebig	Espironolactona	191163001	1
Fiebig	Espironolactona	19h23-b06-194567	1
Fiebig	Espironolactona	B06-1945607	1
Gehe	Espironolactona	12049105	1
Gehe	Espironolactona	13D12-N08	1
GEHE	Espironolactona	16077325	1
gehe	Espironolactona	17E22-B11-335455	1
Gehe	Espironolactona	17H16-B05-341740	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Espironolactona	18208003	1
Gehe	Espironolactona	19015803	1
Gehe	Espironolactona	191163008	1
Gehe	Espironolactona	21000085010	1
Jenne	Espironolactona	14378715	1
Kehr	Espironolactona	22000904008	1
Kehr	Espironolactona	22000904012	1
Noweda/ Caesar&Loren...	Espironolactona	18208008	1
Noweda	Espironolactona	1101013-0	1
Noweda	Espironolactona	14378710	1
Noweda	Espironolactona	1504016-01	1
Noweda	Espironolactona	1602006-01	1
Noweda	Espironolactona	1612002-01	1
noweda	Espironolactona	16A14-B05-525187	1
Noweda	Espironolactona	19H23-B06-194245	1
Noweda	Espironolactona	21000085017	1
Noweda	Espironolactona	22000904012	1
Noweda	Espironolactona	22000904013	2
Noweda	Espironolactona	2203010-01	3
Noweeda	Espironolactona	22000904005	1
Phoenix	Espironolactona	1612002-01	2
Phoenix	Espironolactona	18208008	1
Phoenix	Espironolactona	18A24-B03-354314	1
Phoenix	Espironolactona	19C29-B06-191465	1
Phoenix	Espironolactona	19H23-B06-1942405	2
Phönix	Espironolactona	1101013-03	1
Phönix	Espironolactona	17H16-B05-344771	1
Phönix	Espironolactona	1809020-01	2
Phönix	Espironolactona	18208003	1
Phönix	Espironolactona	18208004	1
Phönix	Espironolactona	191163002	3
Phönix	Espironolactona	20003886005	2
Phönix	Espironolactona	2006012-01	1
Phönix	Espironolactona	21000085007	1
Sanacorp/Phoenix	Espironolactona	13124315	2
Sanacorp	Espironolactona	11042612	1
Sanacorp	Espironolactona	12049103	2
Sanacorp	Espironolactona	12049130	1
Sanacorp	Espironolactona	1212034-01	1
Sanacorp	Espironolactona	13124304	1
Sanacorp	Espironolactona	13124315	1
Sanacorp	Espironolactona	16077325	2
Sanacorp	Espironolactona	18004913	1
Sanacorp	Espironolactona	18208004	1
Sanacorp	Espironolactona	19H23-B06-194567	1
Sanacorp	Espironolactona	20003886005	1
Sanacorp	Espironolactona	22000904018	1
Sanacorp	Espironolactona	23001294006	1
Sanacorp	Espironolactona	9330610	1
WE Phönix 25.11..201...	Espironolactona	16077303	1
Zhejiang Langhua /Phönix	Espironolactona	18004917	2
Zhejiang Langhua /Phönix	Espironolactona	18208003	1
Zhejiang Langhua Pha...	Espironolactona	Q3312	1
Zhejiang/Phoenix	Espironolactona	OT00E1902002	1

- 234 788 spectra from 1515 *Apo-Ident* customers from a total of 49 022 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Espironolactona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Espironolactona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	470	0	152 492
Type B	0	736	0	201 348
Type C	0	1177	102	234 788

The substance/substance group *Espironolactona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7234 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1848 %)
Type C	100.0000 % (> 99.9007 %)	92.0250 % (> 91.7905 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21032	21032	0,00	122,45
21076	21032	4,34	118,67
22369	22369	0,00	127,05
22385	22369	6,66	116,97
22386	22444	5,26	116,88
22444	22444	0,00	117,29
22942	22369	3,81	121,09
24548	24548	0,00	116,91
25213	25213	0,00	112,40
25311	25311	0,00	123,57

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estearato de magnésio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20707-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estearato de magnésio; Magnesii stearas

Special notes

When selecting the *Estearato de magnésio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estearato de magnésio	7	10	34

Second-stage model

For differentiation of the substance/substance group *Estearato de magnésio* the following second-stage model is used:

- Submodelo 01

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estearato de magnésio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Palmitato de cetila	51,79	15,37
⋮	⋮	⋮
Cera de abelha, branca	>50	19,46
Base para supositório (Witepsol W35)	>50	20,81
Gordura sólida	>50	22,16
Parafina sólida	>50	25,83
Cera de abelha, amarela	>50	29,49
Manteiga de cacau	>50	32,14
Parafina, microcristalina	>50	36,27
Dodecilsulfato de sódio	>50	40,52

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estearato de magnésio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Estearato de magnésio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estearato de magnésio	13095536	21117	40	20130405
Caelo	Estearato de magnésio	14136929	21783	60	AR-15-FG-012028-01
Euro OTC	Estearato de magnésio	1502033-01	22817	40	20150317
Euro OTC	Estearato de magnésio	1704002	23436	40	20170622*
Euro OTC	Estearato de magnésio	2301035	26649	40	20230323*
Euro OTC	Estearato de magnésio	2301035	26649SI	20	20230323*
Fagron	Estearato de magnésio	12C29-N06	20707	110	20120418
Fagron	Estearato de magnésio	12D26-B03	21084	40	1407310

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 390 spectra of 8 reference samples from the substance/substance group *Estearato de magnésio*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 572 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 12 reference samples from the substance/substance group *Estearato de magnésio*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estearato de magnésio	162066	22763	40
Caelo	Estearato de magnésio	181533	24215	40
Caelo	Estearato de magnésio	183089	24354	40
Caelo	Estearato de magnésio	192527	24897	40
Caelo	Estearato de magnésio	21004078013	26743	40
Caelo	Estearato de magnésio	23002099	26973	40
Euro OTC	Estearato de magnésio	1608022	22821	40
Euro OTC	Estearato de magnésio	1901033	24459	40
Euro OTC	Estearato de magnésio	2009032	25398	40
Euro OTC	Estearato de magnésio	2109010	25886	50
Caelo	Estearato de magnésio	21004078013	26743SI	20
Euro OTC	Estearato de magnésio	2109010	25886SI	10

- 201 644 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 65 spectra from 48 *Apo-Ident* customers from 36 batches from the substance/substance group *Estearato de magnésio*.
- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estearato de magnésio	21004078005	1
	Estearato de magnésio	2100407813	1
	Estearato de magnésio	23000572003	2
Caelo	Estearato de magnésio	12040307	1
Caelo	Estearato de magnésio	13095515	1
Caelo	Estearato de magnésio	13095536	1
Caelo	Estearato de magnésio	15155001	2
Caelo	Estearato de magnésio	15305302	3
Caelo	Estearato de magnésio	15305307	1
Caelo	Estearato de magnésio	15305315	4
Caelo	Estearato de magnésio	15305323	1
Caelo	Estearato de magnésio	16206602	3
Caelo	Estearato de magnésio	16206610	7
Caelo	Estearato de magnésio	16206617	1
Caelo	Estearato de magnésio	17360006	2
Caelo	Estearato de magnésio	18153310	2
Caelo	Estearato de magnésio	183038912	1
Caelo	Estearato de magnésio	18308912	1
Caelo	Estearato de magnésio	18308916	2
Caelo	Estearato de magnésio	192527003	1
Caelo	Estearato de magnésio	192527006	1
Caelo	Estearato de magnésio	20004065001	2
Caesar & Loretz GmbH...	Estearato de magnésio	15322002	1
Caesar & Loretz GmbH/Kehr	Estearato de magnésio	18153310	1
Caesar & Loretz GmbH...	Estearato de magnésio	18153310	1
Caesar & Loretz GmbH	Estearato de magnésio	18308912	1
Caesar & Loretz GmbH	Estearato de magnésio	18308916	1
Caesar & Loretz GmbH	Estearato de magnésio	192527003	1
Caesar & Loretz GmbH	Estearato de magnésio	20004065001	1
Euro OTC	Estearato de magnésio	1116E-01834	1
Euro OTC	Estearato de magnésio	1119I-01834	1
Euro OTC	Estearato de magnésio	1502033-01	2
Euro OTC	Estearato de magnésio	1912I-01834	1
Euro OTC	Estearato de magnésio	2009032-01	1
Euro OTC	Estearato de magnésio	315E-01834	1
Euro OTC	Estearato de magnésio	718I-01834	1
Euro OTC	Estearato de magnésio	914I-01834	1
Fagron	Estearato de magnésio	12D26-B03-289435	1
FL Apotheke	Estearato de magnésio	xxxxxx	1
Jenne	Estearato de magnésio	21004078010	1
Noweda	Estearato de magnésio	21004078013	1
Phoenix	Estearato de magnésio	23000572003	1
ROHA	Estearato de magnésio	130230	1
Sanacorp	Estearato de magnésio	21004078013	1
Sanacorp	Estearato de magnésio	23000572003	1

- 236 002 spectra from 1515 *Apo-Ident* customers from a total of 49 223 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estearato de magnésio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estearato de magnésio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	390	0	152 572
Type B	0	440	0	201 644
Type C	0	65	0	236 002

The substance/substance group *Estearato de magnésio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4615 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.7692 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20707	21783	54,93	106,34
21084	21084	0,00	134,05
21117	26649	26,21	129,88
21783	21783	0,00	139,76
22817	21783	5,71	139,16
23436	23436	0,00	133,97
26649	26649	0,00	132,63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estearato de zinco**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24018-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estearato de zinco; Zinci stearas

Special notes

When selecting the *Estearato de zinco* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estearato de zinco	2	1	1

Second-stage model

For differentiation of the substance/substance group *Estearato de zinco* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estearato de zinco* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Palmitato de cetila	33,14	–
Cera de abelha, branca	35,94	–
Parafina sólida	37,98	–
Cera de abelha, amarela	38,21	–
Gordura sólida	50,80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estearato de zinco* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Estearato de zinco*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estearato de zinco	180628	24018	40	20180322*
Caelo	Estearato de zinco	22000651	26123	40	20220426*
Caelo	Estearato de zinco	22000651	26123SI	20	20220426*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 100 spectra of 3 reference samples from the substance/substance group *Estearato de zinco*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 862 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Estearato de zinco*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estearato de zinco	182279	24500	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Estearato de zinco*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estearato de zinco	22002130001	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estearato de zinco* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estearato de zinco* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	40	0	202 044
Type C	0	1	0	236 066

The substance/substance group *Estearato de zinco* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24018	24018	0,00	46,43
26123	26123	0,00	43,85

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estradiol hemi-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20497-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estradiol hemi-hidratado; Estradiolum hemihydricum

Special notes

When selecting the *Estradiol hemi-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estradiol hemi-hidratado	11	27	155

Second-stage model

For differentiation of the substance/substance group *Estradiol hemi-hidratado* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estradiol hemi-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	52,45	–
⋮	⋮	⋮
Estriol	>50	20,42
Sulfato de polimixina B	>50	36,54
Bacitracina	>50	41,95
Anfotericina B	>50	53,77
Cianocobalamina	>50	56,99
Riboflavina	>50	58,27
Sulfato de colistina	>50	59,92
Nistatina	>50	72,43
Triancinolona	>50	73,96
Vitamina E acetato pó 50%	>50	101,15
Glicerofosfato de cálcio	>50	110,81
Levedura de selênio	>50	127,57
Metilcobalamina	>50	135,87
Pantotenato de cálcio	>50	137,78
Gelatina, branca	>50	164,68
SyrSpend® SF Alka	>50	185,24
Bromidrato de hioscina	>50	194,33
Tosilcloramida sódica	>50	201,04
SyrSpend® SF pH4 neo	>50	211,67
Carmelose sódica	>50	220,24
Amido de arroz	>50	298,95
Ácido oxálico	>50	338,81
Amido de milho	>50	347,66
Goma arábica, dispersão seca	>50	498,96
Amido de trigo	>50	507,84
SyrSpend® SF pH4	>50	508,23
Maltodextrina	>50	533,89
Fécula de batata	>50	594,92
Frutose	>50	715,93

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estradiol hemi-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Estradiol hemi-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estradiol hemi-hidratado	12268016	21302	40	1410502
Caelo	Estradiol hemi-hidratado	13285802	21499	60	20130913
Caelo	Estradiol hemi-hidratado	13285802	21500	60	1510622
Caelo	Estradiol hemi-hidratado	13285802	21501	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21502	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21503	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21504	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21505	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21506	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21507	20	20130913
Caelo	Estradiol hemi-hidratado	13285802	21508	60	1410504
Euro OTC	Estradiol hemi-hidratado	1208022-01	21291	40	20121012
Euro OTC	Estradiol hemi-hidratado	1507013	21847	60	1510623
Euro OTC	Estradiol hemi-hidratado	1507013	21847SI	60	1510623
Euro OTC	Estradiol hemi-hidratado	1510039	21945	60	20151103*
Euro OTC	Estradiol hemi-hidratado	1510039	21945SI	89	20151103*
Euro OTC	Estradiol hemi-hidratado	1601017	22307	45	20160122*
Euro OTC	Estradiol hemi-hidratado	1612008	22913	40	20170117*
Euro OTC	Estradiol hemi-hidratado	1612008	22913SI	40	20170117*
Euro OTC	Estradiol hemi-hidratado	2009029	25402	40	20201012*
Euro OTC	Estradiol hemi-hidratado	2103014	25608	40	20210406*
Euro OTC	Estradiol hemi-hidratado	2103014	25608SI	40	20210406*
Fagron	Estradiol hemi-hidratado	14G24-B04-297404	21667	55	20140825
Fagron	Estradiol hemi-hidratado	16H04-B01-328738	23184	40	20160915

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1009 spectra of 24 reference samples from the substance/substance group *Estradiol hemi-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 151 953 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2464 spectra of 65 reference samples from the substance/substance group *Estradiol hemi-hidratado*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estradiol hemi-hidratado	170582	23339	40
Caelo	Estradiol hemi-hidratado	181443	24257	40
Caelo	Estradiol hemi-hidratado	21003879006	26315	40
Euro OTC	Estradiol hemi-hidratado	1607003	22712	40
Euro OTC	Estradiol hemi-hidratado	1612008-01	23099	40
Euro OTC	Estradiol hemi-hidratado	1705018	23431	40
Euro OTC	Estradiol hemi-hidratado	1710031	23779	40
Euro OTC	Estradiol hemi-hidratado	1802013	24083	40
Euro OTC	Estradiol hemi-hidratado	1802012	24086	40
Euro OTC	Estradiol hemi-hidratado	1809022	24319	40
Euro OTC	Estradiol hemi-hidratado	1808032	24322	40
Euro OTC	Estradiol hemi-hidratado	1905001	24639	40
Euro OTC	Estradiol hemi-hidratado	1906013	24772	40
Euro OTC	Estradiol hemi-hidratado	1910006	24973	40
Euro OTC	Estradiol hemi-hidratado	1911010	24983	40
Euro OTC	Estradiol hemi-hidratado	2002008	25108	40
Euro OTC	Estradiol hemi-hidratado	2002009	25109	40
Euro OTC	Estradiol hemi-hidratado	2002007	25114	40
Euro OTC	Estradiol hemi-hidratado	2006023	25257	40
Euro OTC	Estradiol hemi-hidratado	2006024	25266	40
Euro OTC	Estradiol hemi-hidratado	2006022	25284	40
Euro OTC	Estradiol hemi-hidratado	2009028	25403	40
Euro OTC	Estradiol hemi-hidratado	2201041	25966	40
Euro OTC	Estradiol hemi-hidratado	2303010	26656	40
Euro OTC	Estradiol hemi-hidratado	2405012	27278	40
Fagron	Estradiol hemi-hidratado	13K22-N01	21263	40
Fagron	Estradiol hemi-hidratado	22I23-B01-225111	26374	40
Caelo	Estradiol hemi-hidratado	13285802	21499SI†	60
Caelo	Estradiol hemi-hidratado	13285802	21500SI†	60
Caelo	Estradiol hemi-hidratado	13285802	21501SI†	20
Caelo	Estradiol hemi-hidratado	13285802	21502SI†	20
Caelo	Estradiol hemi-hidratado	13285802	21503SI†	20
Caelo	Estradiol hemi-hidratado	13285802	21504SI†	20
Caelo	Estradiol hemi-hidratado	13285802	21505SI†	20
Caelo	Estradiol hemi-hidratado	13285802	21506SI†	20
Caelo	Estradiol hemi-hidratado	13285802	21507SI†	20
Caelo	Estradiol hemi-hidratado	170582	23339SI	30
Caelo	Estradiol hemi-hidratado	181443	24257SI	40
Caelo	Estradiol hemi-hidratado	21003879006	26315SI	40
Euro OTC	Estradiol hemi-hidratado	1601017	22307SI†	45
Euro OTC	Estradiol hemi-hidratado	1607003	22712SI	40
Euro OTC	Estradiol hemi-hidratado	1612008-01	23099SI	30
Euro OTC	Estradiol hemi-hidratado	1705018	23431SI	30
Euro OTC	Estradiol hemi-hidratado	1710031	23779SI	40

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Estradiol hemi-hidratado	1802013	24083SI	40
Euro OTC	Estradiol hemi-hidratado	1802012	24086SI	40
Euro OTC	Estradiol hemi-hidratado	1809022	24319SI	40
Euro OTC	Estradiol hemi-hidratado	1808032	24322SI	40
Euro OTC	Estradiol hemi-hidratado	1905001	24639SI	40
Euro OTC	Estradiol hemi-hidratado	1906013	24772SI	39
Euro OTC	Estradiol hemi-hidratado	1910006	24973SI	40
Euro OTC	Estradiol hemi-hidratado	1911010	24983SI	40
Euro OTC	Estradiol hemi-hidratado	2002008	25108SI	40
Euro OTC	Estradiol hemi-hidratado	2002009	25109SI	40
Euro OTC	Estradiol hemi-hidratado	2002007	25114SI	40
Euro OTC	Estradiol hemi-hidratado	2006023	25257SI	40
Euro OTC	Estradiol hemi-hidratado	2006024	25266SI	40
Euro OTC	Estradiol hemi-hidratado	2006022	25284SI	40
Euro OTC	Estradiol hemi-hidratado	2009029	25402SI†	40
Euro OTC	Estradiol hemi-hidratado	2009028	25403SI	40
Euro OTC	Estradiol hemi-hidratado	2201041	25966SI	40
Euro OTC	Estradiol hemi-hidratado	2303010	26656SI	40
Euro OTC	Estradiol hemi-hidratado	2405012	27278SI	40
Fagron	Estradiol hemi-hidratado	16H04-B01-328738	23184SI†	30
Fagron	Estradiol hemi-hidratado	22I23-B01-225111	26374SI	40

- 199 620 spectra from a total of 4014 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 597 spectra from 220 *Apo-Ident* customers from 164 batches from the substance/substance group *Estradiol hemi-hidratado*.

- Among them are spectra of independent samples from 155 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estradiol hemi-hidratado	21003879006	2
	Estradiol hemi-hidratado	21003879009	2
	Estradiol hemi-hidratado	2103014-02	1
	Estradiol hemi-hidratado	22123-B01	1
	Estradiol hemi-hidratado	23000120001	2
	Estradiol hemi-hidratado	2300020001	1
Anzag; 12.72EUR; 7.10.2015	Estradiol hemi-hidratado	15038004	1
Audor Pharma	Estradiol hemi-hidratado	1911010-01	1
Bayer Pharma AG	Estradiol hemi-hidratado	1411024-01	2
Caelo	Estradiol hemi-hidratado	108082101	1
Caelo	Estradiol hemi-hidratado	11078104	1
Caelo	Estradiol hemi-hidratado	11078105	1
Caelo	Estradiol hemi-hidratado	11078113	1
Caelo	Estradiol hemi-hidratado	12172003	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estradiol hemi-hidratado	12268003	1
Caelo	Estradiol hemi-hidratado	12268012	5
Caelo	Estradiol hemi-hidratado	12F29-N03	1
Caelo	Estradiol hemi-hidratado	13285801	1
Caelo	Estradiol hemi-hidratado	13285802	4
Caelo	Estradiol hemi-hidratado	13285804	1
Caelo	Estradiol hemi-hidratado	13285811	4
Caelo	Estradiol hemi-hidratado	13K22-N01	1
Caelo	Estradiol hemi-hidratado	15038004	5
Caelo	Estradiol hemi-hidratado	1503801	1
Caelo	Estradiol hemi-hidratado	15038010	2
Caelo	Estradiol hemi-hidratado	15038014	2
Caelo	Estradiol hemi-hidratado	15038016	2
Caelo	Estradiol hemi-hidratado	15385406	1
Caelo	Estradiol hemi-hidratado	15385410	4
Caelo	Estradiol hemi-hidratado	15385411	1
Caelo	Estradiol hemi-hidratado	15385415	2
Caelo	Estradiol hemi-hidratado	15D01-B02-319032	1
Caelo	Estradiol hemi-hidratado	1601017-01	5
Caelo	Estradiol hemi-hidratado	1612008-01	1
Caelo	Estradiol hemi-hidratado	17058205	4
Caelo	Estradiol hemi-hidratado	18082101	3
Caelo	Estradiol hemi-hidratado	18082101P-180904-1	1
Caelo	Estradiol hemi-hidratado	18082103	1
Caelo	Estradiol hemi-hidratado	18082104	4
Caelo	Estradiol hemi-hidratado	18082105	6
Caelo	Estradiol hemi-hidratado	18144306	2
Caelo	Estradiol hemi-hidratado	18144308	1
Caelo	Estradiol hemi-hidratado	18144309	3
Caelo	Estradiol hemi-hidratado	18144314	3
Caelo	Estradiol hemi-hidratado	18F18-B01-351946	1
Caelo	Estradiol hemi-hidratado	19051501	1
Caelo	Estradiol hemi-hidratado	193089002	3
Caelo	Estradiol hemi-hidratado	193089003	1
Caelo	Estradiol hemi-hidratado	193089007	5
Caelo	Estradiol hemi-hidratado	193089010	5
Caelo	Estradiol hemi-hidratado	193089011	2
Caelo	Estradiol hemi-hidratado	19308910	1
Caelo	Estradiol hemi-hidratado	20I18-F03-374511	1
Caelo	Estradiol hemi-hidratado	21000148001	7
Caelo	Estradiol hemi-hidratado	21003879001	1
Caelo	Estradiol hemi-hidratado	21003879006	3
Caelo	Estradiol hemi-hidratado	22101301	1
Caelo	Estradiol hemi-hidratado	84201560	1
Caelo	Estradiol hemi-hidratado	9248916	2
Caesar & Loretz GmbH...	Estradiol hemi-hidratado	18144309	1
Caesar & Loretz GmbH...	Estradiol hemi-hidratado	21003879006	1
Caesar & Loretz GmbH...	Estradiol hemi-hidratado	193089011	1
Caesar & Loretz GmbH/Sana	Estradiol hemi-hidratado	193089010	1
Caesar & Loretz GmbH...	Estradiol hemi-hidratado	193089011	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	15385415	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	18082104	5
Caesar & Loretz GmbH	Estradiol hemi-hidratado	18082105	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	18144306	2
Caesar & Loretz GmbH	Estradiol hemi-hidratado	18144309	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	193089002	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	193089006	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	193089007	2
Caesar & Loretz GmbH	Estradiol hemi-hidratado	193089011	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	21000148001	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estradiol hemi-hidratado	21000148003	1
Caesar & Loretz GmbH	Estradiol hemi-hidratado	21003879006	5
ESD	Estradiol hemi-hidratado	ESD-20010	1
EuRho/Sanacorp	Estradiol hemi-hidratado	1911010-01	1
Eurho	Estradiol hemi-hidratado	2002007-01	1
Euro OTC	Estradiol hemi-hidratado	1308003-01	2
Euro OTC	Estradiol hemi-hidratado	1374814	1
Euro OTC	Estradiol hemi-hidratado	1404030-01	1
Euro OTC	Estradiol hemi-hidratado	1411024-01	2
Euro OTC	Estradiol hemi-hidratado	1504034-01	1
Euro OTC	Estradiol hemi-hidratado	1507013-01	1
Euro OTC	Estradiol hemi-hidratado	1510039-01	11
Euro OTC	Estradiol hemi-hidratado	15D01-B02	1
Euro OTC	Estradiol hemi-hidratado	1601017-01	10
Euro OTC	Estradiol hemi-hidratado	1607003-01	29
Euro OTC	Estradiol hemi-hidratado	1607003-0101374814	1
Euro OTC	Estradiol hemi-hidratado	1612008_01	1
Euro OTC	Estradiol hemi-hidratado	1612008-01	26
Euro OTC	Estradiol hemi-hidratado	1705018-01	21
Euro OTC	Estradiol hemi-hidratado	17058205	1
Euro OTC	Estradiol hemi-hidratado	1802012-01	1
Euro OTC	Estradiol hemi-hidratado	1802013-01	3
Euro OTC	Estradiol hemi-hidratado	1808032-01	23
Euro OTC	Estradiol hemi-hidratado	1809022-01	7
Euro OTC	Estradiol hemi-hidratado	180902202	1
Euro OTC	Estradiol hemi-hidratado	1809022-02	6
Euro OTC	Estradiol hemi-hidratado	1906013-01	3
Euro OTC	Estradiol hemi-hidratado	1910006-01	4
Euro OTC	Estradiol hemi-hidratado	1911010-01	4
Euro OTC	Estradiol hemi-hidratado	2002009-01	4
Euro OTC	Estradiol hemi-hidratado	2006022-01	15
Euro OTC	Estradiol hemi-hidratado	2006023-01	12
Euro OTC	Estradiol hemi-hidratado	2006024-01	14
Euro OTC	Estradiol hemi-hidratado	20090028-01	1
Euro OTC	Estradiol hemi-hidratado	2009028-01	18
Euro OTC	Estradiol hemi-hidratado	2009029	10
Euro OTC	Estradiol hemi-hidratado	2009029-01	20
Euro OTC	Estradiol hemi-hidratado	2103014-0	2
Euro OTC	Estradiol hemi-hidratado	210301401	1
Euro OTC	Estradiol hemi-hidratado	2103014-01	19
Euro OTC	Estradiol hemi-hidratado	2201041-01	8
Euro OTC	Estradiol hemi-hidratado	2303010-01	6
Euro OTC	Estradiol hemi-hidratado	2405012-01	1
Euro OTC	Estradiol hemi-hidratado	27061714	1
Euro OTC	Estradiol hemi-hidratado	701634	1
Euro/ Phönix	Estradiol hemi-hidratado	3417M-02845	1
Fagron	Estradiol hemi-hidratado		1
Fagron	Estradiol hemi-hidratado	11031401	1
Fagron	Estradiol hemi-hidratado	11A21-N01	1
Fagron	Estradiol hemi-hidratado	11H23-N02	1
Fagron	Estradiol hemi-hidratado	12F29-N03	6
Fagron	Estradiol hemi-hidratado	12L19-N07	7
Fagron	Estradiol hemi-hidratado	12L29-N07	1
Fagron	Estradiol hemi-hidratado	13E07-N02	4
Fagron	Estradiol hemi-hidratado	13k22n01	1
Fagron	Estradiol hemi-hidratado	13K22N01	1
Fagron	Estradiol hemi-hidratado	13K22-N01	7
Fagron	Estradiol hemi-hidratado	14G24-B04	1
Fagron	Estradiol hemi-hidratado	14G24-B04-297402	3
Fagron	Estradiol hemi-hidratado	14G24-B04-297404	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Estradiol hemi-hidratado	14G24-B04-297405	1
Fagron	Estradiol hemi-hidratado	14G24-B04-297406	1
Fagron	Estradiol hemi-hidratado	14G24-B04-302446	3
Fagron	Estradiol hemi-hidratado	15D01-B02-308190	1
Fagron	Estradiol hemi-hidratado	15D01-B02-308568	2
Fagron	Estradiol hemi-hidratado	15D01-B02-312068	3
Fagron	Estradiol hemi-hidratado	15D01-B02-319032	4
Fagron	Estradiol hemi-hidratado	16D12-B01-322022	1
Fagron	Estradiol hemi-hidratado	16D12B01326783	1
Fagron	Estradiol hemi-hidratado	16D12-B01-326783	6
Fagron	Estradiol hemi-hidratado	16h04-b01-328738	1
Fagron	Estradiol hemi-hidratado	16H04-B01-328738	1
Fagron	Estradiol hemi-hidratado	16h04-b01-334200	1
Fagron	Estradiol hemi-hidratado	16H04-B01-334200	4
Fagron	Estradiol hemi-hidratado	16H04-B01-334592	1
Fagron	Estradiol hemi-hidratado	16h04-b01-337595	1
Fagron	Estradiol hemi-hidratado	16H04-B01-33795	1
Fagron	Estradiol hemi-hidratado	16H04-B01-339490	1
Fagron	Estradiol hemi-hidratado	1802012-01	1
Fagron	Estradiol hemi-hidratado	1802013-01	3
Fagron	Estradiol hemi-hidratado	18F18-B01	2
Fagron	Estradiol hemi-hidratado	18F18-B01-351789	1
Fagron	Estradiol hemi-hidratado	18F18-B01-351790	1
Fagron	Estradiol hemi-hidratado	18F18-B01-351946	2
Fagron	Estradiol hemi-hidratado	18F18-B01-354821	1
Fagron	Estradiol hemi-hidratado	18F18-B01-355586	1
Fagron	Estradiol hemi-hidratado	18F18-B01-357641	2
Fagron	Estradiol hemi-hidratado	18F18-B01-359015	2
Fagron	Estradiol hemi-hidratado	18F18B01360269	1
Fagron	Estradiol hemi-hidratado	18F18-B01-360269	1
Fagron	Estradiol hemi-hidratado	18F18-B01-363586	3
Fagron	Estradiol hemi-hidratado	18F18-B01-363587	2
Fagron	Estradiol hemi-hidratado	20B07-F02-369198	1
Fagron	Estradiol hemi-hidratado	20b07-f02-369199	1
Fagron	Estradiol hemi-hidratado	20B07-F02-369529	1
Fagron	Estradiol hemi-hidratado	20I18-F03-374511	1
Fagron	Estradiol hemi-hidratado	20I18-F03-374511	2
Fagron	Estradiol hemi-hidratado	20l18-F03-374511	1
Fagron	Estradiol hemi-hidratado	21E12-F07-378251	2
Fagron	Estradiol hemi-hidratado	21E12-F07-378252	1
Fagron	Estradiol hemi-hidratado	21E12-F07-378866	2
Fagron	Estradiol hemi-hidratado	302446	1
Fagron	Estradiol hemi-hidratado	83100820	2
Fagron	Estradiol hemi-hidratado	84201170	1
Fagron	Estradiol hemi-hidratado	84201560	1
Fagron	Estradiol hemi-hidratado	9G07N01	1
Fagron	Estradiol hemi-hidratado	9J27-N05	1
Fagron	Estradiol hemi-hidratado	F02-3695209	1
Fagron	Estradiol hemi-hidratado	UN80044	1
Fargon	Estradiol hemi-hidratado	2B07-369198	1
Fargon	Estradiol hemi-hidratado	B01-3635806	1
Fargon	Estradiol hemi-hidratado	f02-3691908	1
Fargron/ Sanacorp	Estradiol hemi-hidratado	14G24-b04-297402	1
Fiebig	Estradiol hemi-hidratado	16H04-B01	1
Gatt-Koller	Estradiol hemi-hidratado	1801604	2
Gehe	Estradiol hemi-hidratado	15038016	1
Gehe	Estradiol hemi-hidratado	82404160	1
Henry Lamotte/AHD	Estradiol hemi-hidratado	18082101	1
La Chandra /Noweda	Estradiol hemi-hidratado	210301401	1
Noweda	Estradiol hemi-hidratado	12268008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Estradiol hemi-hidratado	15038004	1
Noweda	Estradiol hemi-hidratado	18F18-B01_351946	1
Noweda	Estradiol hemi-hidratado	21003879006	1
phönix	Estradiol hemi-hidratado	13285802	1
Phönix	Estradiol hemi-hidratado	21003879002	1
Phönix	Estradiol hemi-hidratado	21003879009	3
Phönix	Estradiol hemi-hidratado	23000120001	1
Röntgen	Estradiol hemi-hidratado	18082105	1
Röntgen	Estradiol hemi-hidratado	193089002	1
Sanacorp /Fargron	Estradiol hemi-hidratado	15D01-B02-312068	1
Sanacorp	Estradiol hemi-hidratado	15038010	1
Sanacorp	Estradiol hemi-hidratado	18F18-B01	1
Sanacorp	Estradiol hemi-hidratado	21E12-F07-379952	2
Symbiotec/Phoenix	Estradiol hemi-hidratado	20/18-F03	1
vDL	Estradiol hemi-hidratado	2103014-02	1

- 235 470 spectra from 1515 *Apo-Ident* customers from a total of 49 094 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estradiol hemi-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estradiol hemi-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	1009	0	151 953
Type B	0	2464	0	199 620
Type C	0	596	1	235 470

The substance/substance group *Estradiol hemi-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4054 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.7565 %)
Type C	100.0000 % (> 99.9007 %)	99.8325 % (> 99.3300 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21291	21945	4,81	107,01
21302	21302	0,00	122,09
21499	21847	6,45	102,43
21500	21500	0,00	96,67
21501	21302	5,59	117,90
21502	21302	5,71	116,43
21503	21302	10,98	116,31
21504	21302	6,78	117,31
21505	21302	9,73	116,01
21506	21945	9,63	110,18
21507	21302	5,80	120,88
21508	21508	0,00	126,71
21667	21945	2,93	108,78
21847	21847	0,00	102,68
21945	21945	0,00	111,18
22307	22307	0,00	114,66
22913	22913	0,00	115,65
23184	22307	4,15	118,79
25402	25402	0,00	116,96
25608	25608	0,00	113,33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estriol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20878-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estriol; Estriolum

Special notes

When selecting the *Estriol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estriol	8	19	195

Second-stage model

For differentiation of the substance/substance group *Estriol* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estriol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	59,24	–
⋮	⋮	⋮
Sulfato de polimixina B	>50	36,89
Bacitracina	>50	55,12
Estradiol hemi-hidratado	>50	55,51
Riboflavina	>50	79,05
Sulfato de colistina	>50	79,33
Anfotericina B	>50	85,38
Cianocobalamina	>50	120,17
Triancinolona	>50	128,67
Pantotenato de cálcio	>50	135,64
Nistatina	>50	148,75
Vitamina E acetato pó 50%	>50	176,15
Levedura de selênio	>50	201,07
Tosilcloramida sódica	>50	203,77
Bromidrato de hioscina	>50	222,98
Metilcobalamina	>50	226,25
Glicerofosfato de cálcio	>50	237,35
Gelatina, branca	>50	264,73
Carmelose sódica	>50	342,14
SyrSpend® SF pH4 neo	>50	413,17
SyrSpend® SF Alka	>50	416,35
Ácido oxálico	>50	420,81
Amido de arroz	>50	554,85
Amido de milho	>50	634,93
Amido de trigo	>50	662,17
Goma arábica, dispersão seca	>50	665,64
Maltodextrina	>50	862,70
SyrSpend® SF pH4	>50	888,58
Fécula de batata	>50	919,78
Frutose	>50	1031,11

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estriol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance/substance group *Estriol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estriol	12298706	20878	40	20121106
Caelo	Estriol	13256001	21390	55	1511155
Caelo	Estriol	13256001	21390SI	60	1511155
Caelo	Estriol	13256001	21391	60	20130821
Caelo	Estriol	13256001	21392	20	20130821
Caelo	Estriol	13256001	21393	60	20130821
Caelo	Estriol	13256001	21394	20	20130821
Caelo	Estriol	13256001	21395	20	20130821
Caelo	Estriol	13256001	21399	20	20130821
Caelo	Estriol	13256001	21400	20	20130821
Caelo	Estriol	13256001	21401	20	20130821
Caelo	Estriol	13256001	21404	20	20130821
Euro OTC	Estriol	1507026	21848	60	0000010671
Euro OTC	Estriol	1507026	21848SI	60	0000010671
Euro OTC	Estriol	1509042	21939	60	20151009*
Euro OTC	Estriol	1509042	21939SI	60	20151009*
Euro OTC	Estriol	1703044	23181	40	20170502*
Fagron	Estriol	11J13-N07	21255	40	1412180
Fagron	Estriol	16D15-B03-322957	22889	40	20160711
Fagron	Estriol	16D15-B03-322957	22889SI	40	20160711
Fagron	Estriol	16I19-B01-331468	23172	40	20170301

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 855 spectra of 21 reference samples from the substance/substance group *Estriol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.
- 152 107 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 1777 spectra of 47 reference samples from the substance/substance group *Estriol*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estriol	161382	22633	40
Caelo	Estriol	2010002	25400	40
Caelo	Estriol	22003580	26715	39
Euro OTC	Estriol	1310002-01	21292	40
Euro OTC	Estriol	1606044	22711	40
Euro OTC	Estriol	1610035	22850	40
Euro OTC	Estriol	1710022	23731	40
Euro OTC	Estriol	1710030	23733	40
Euro OTC	Estriol	1803011	24073	40
Euro OTC	Estriol	1903035	24604	40
Euro OTC	Estriol	2002010	25107	40
Euro OTC	Estriol	2007001	25237	40
Euro OTC	Estriol	2103007	25610	40
Euro OTC	Estriol	2107006	25706	50
Euro OTC	Estriol	2111005	25884	50
Euro OTC	Estriol	2302018	26660	40
Euro OTC	Estriol	2312004	27158	39
Euro OTC	Estriol	2402025	27286	40
Fagron	Estriol	22H12-B05-224456	26455	40
Caelo	Estriol	13256001	21391SI†	60
Caelo	Estriol	13256001	21392SI†	20
Caelo	Estriol	13256001	21394SI†	20
Caelo	Estriol	13256001	21395SI†	20
Caelo	Estriol	13256001	21399SI†	20
Caelo	Estriol	13256001	21400SI†	20
Caelo	Estriol	13256001	21401SI†	20
Caelo	Estriol	13256001	21404SI†	20
Caelo	Estriol	161382	22633SI	40
Caelo	Estriol	2010002	25400SI	40
Caelo	Estriol	22003580	26715SI	40
Euro OTC	Estriol	1606044	22711SI	40
Euro OTC	Estriol	1610035	22850SI	40
Euro OTC	Estriol	1703044	23181SI†	40
Euro OTC	Estriol	1710022	23731SI	40
Euro OTC	Estriol	1710030	23733SI	40
Euro OTC	Estriol	1803011	24073SI	40
Euro OTC	Estriol	1903035	24604SI	40
Euro OTC	Estriol	2002010	25107SI	40
Euro OTC	Estriol	2007001	25237SI	40
Euro OTC	Estriol	2103007	25610SI	40
Euro OTC	Estriol	2107006	25706SI	50
Euro OTC	Estriol	2111005	25884SI	50
Euro OTC	Estriol	2302018	26660SI	40
Euro OTC	Estriol	2312004	27158SI	30
Euro OTC	Estriol	2402025	27286SI	40
Fagron	Estriol	16I19-B01-331468	23172SI†	30
Fagron	Estriol	22H12-B05-224456	26455SI	39

- 200 307 spectra from a total of 4023 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 628 spectra from 300 *Apo-Ident* customers from 203 batches from the substance/substance group *Estriol*.
- Among them are spectra of independent samples from 185 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estriol	20G10-f06-372935	1
	Estriol	20G10-F06-372935	1
	Estriol	21002272024	1
	Estriol	22003680002	1
	Estriol	22H12-B06-222366	2
	Estriol	23A30-B01-227260	1
	Estriol	23A30-B01-227261	1
	Estriol	B06-2223606	1
	Estriol	L00048288	1
AHD	Estriol	16I19-B01-331466	1
apomix	Estriol	14077904	1
Apotheke am Luisenho...	Estriol	20000085004	2
Audor Pharma	Estriol		16
Audor Pharma	Estriol	2002010-01	1
Audor Pharma	Estriol	AP20780041010218E	1
Audor Pharma	Estriol	AP20780041020218E	3
Audor Pharma	Estriol	APL000036940E	1
Audor Pharma	Estriol	APL00036940E	2
Audor Pharma	Estriol	APL00037293	1
Audor Pharma	Estriol	APL00037293E	1
Aufor/AHD	Estriol		1
Bayer Pharma GmbH / ...	Estriol	15297804	1
Bombastus	Estriol	5128	1
Caelo	Estriol	10053206	1
Caelo	Estriol	10H30-N06	1
Caelo	Estriol	11254402	1
Caelo	Estriol	11254410	1
Caelo	Estriol	11254412	1
Caelo	Estriol	12032503	4
Caelo	Estriol	12032504	2
Caelo	Estriol	12032507	5
Caelo	Estriol	12298702	2
Caelo	Estriol	12298704	6
Caelo	Estriol	12298706	1
Caelo	Estriol	12298707	2
Caelo	Estriol	12H06N02	1
Caelo	Estriol	12H06-N02	1
Caelo	Estriol	13256001	1
Caelo	Estriol	13256004	9
Caelo	Estriol	14077901	1
Caelo	Estriol	14077903	2
Caelo	Estriol	14077904	9
Caelo	Estriol	1409018-01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estriol	14272101	3
Caelo	Estriol	14272104	5
Caelo	Estriol	1477904	1
Caelo	Estriol	14j20-b07	1
Caelo	Estriol	15008902	1
Caelo	Estriol	15028901	4
Caelo	Estriol	15028904	8
Caelo	Estriol	15028905	1
Caelo	Estriol	15297804	17
Caelo	Estriol	15297805	1
Caelo	Estriol	16/19-B01-331467	1
Caelo	Estriol	16053404	1
Caelo	Estriol	16053405	2
Caelo	Estriol	16053408	5
Caelo	Estriol	16053409	1
Caelo	Estriol	16138204	4
Caelo	Estriol	16317701	5
Caelo	Estriol	16317702	6
Caelo	Estriol	16317703	4
Caelo	Estriol	17042014B	1
Caelo	Estriol	1710030-01	2
Caelo	Estriol	17133703	2
Caelo	Estriol	17133704	9
Caelo	Estriol	17133705	4
Caelo	Estriol	17133706	21
Caelo	Estriol	17133709	6
Caelo	Estriol	17133710	8
Caelo	Estriol	17133711	6
Caelo	Estriol	1713373	1
Caelo	Estriol	1733706	1
Caelo	Estriol	17348701	17
Caelo	Estriol	17348702	9
Caelo	Estriol	17348706	10
Caelo	Estriol	17348707	8
Caelo	Estriol	18041811	1
Caelo	Estriol	18247101	4
Caelo	Estriol	19035606	3
Caelo	Estriol	19035607	10
Caelo	Estriol	19035609	2
Caelo	Estriol	200000085004	1
Caelo	Estriol	20000085004	18
Caelo	Estriol	20000085005	1
Caelo	Estriol	20000085006	6
Caelo	Estriol	20G10-F06	1
Caelo	Estriol	20G10-F06-372934	1
Caelo	Estriol	20G10-F06-372958	1
Caelo	Estriol	24031501	1
Caelo	Estriol	27061303	1
Caelo	Estriol	9071801	1
Caelo	Estriol	L00047276	1
Caesar & Loretz GmbH...	Estriol	20000085004	1
Caesar & Loretz GmbH...	Estriol	20000085006	1
Caesar & Loretz GmbH...	Estriol	19035607	1
Caesar & Loretz GmbH...	Estriol	20000085006	1
Caesar & Loretz GmbH...	Estriol	20000085006	1
Caesar & Loretz GmbH	Estriol	15028901	1
Caesar & Loretz GmbH	Estriol	15028904	1
Caesar & Loretz GmbH	Estriol	17133704	1
Caesar & Loretz GmbH	Estriol	17348701	1
Caesar & Loretz GmbH	Estriol	19035607	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estriol	19035609	2
Caesar & Loretz GmbH	Estriol	20000085004	2
Caesar & Loretz GmbH	Estriol	20000085006	2
Caesar & Loretz GmbH	Estriol	21001836002	1
Caesar § Lorenz GmbH	Estriol	12298712	1
Caesar&Loretz,AHC, 1...	Estriol	15297804	1
Cealo/ Sanacorp	Estriol	17133706	2
Cealo/GEHE	Estriol	17348702	1
Ensbona/ Sanacorp	Estriol	16053405	1
EuRho	Estriol	1710030-01	1
Euro OTC	Estriol	1201020-01	1
Euro OTC	Estriol	1310002-01	1
Euro OTC	Estriol	1403011-01	2
Euro OTC	Estriol	1409018-01	1
Euro OTC	Estriol	15028904	1
Euro OTC	Estriol	1507026-01	1
Euro OTC	Estriol	1509042-01	3
Euro OTC	Estriol	1606044-01	14
Euro OTC	Estriol	1610035-01	5
Euro OTC	Estriol	1703044-01	1
Euro OTC	Estriol	170344-01	1
Euro OTC	Estriol	1710030-01	3
Euro OTC	Estriol	17133706	1
Euro OTC	Estriol	1803011-01	1
Euro OTC	Estriol	1903035-01	1
Euro OTC	Estriol	2002010-01	1
Euro OTC	Estriol	2007001-01	6
Euro OTC	Estriol	2010002-01	4
Euro OTC	Estriol	2010002-03	3
Euro OTC	Estriol	2103007-01	7
Euro OTC	Estriol	2107006-01	2
Euro/Phönix	Estriol	1509042-01	1
Fagron	Estriol		2
Fagron	Estriol	11D13-N11	1
Fagron	Estriol	11J13-N07	3
Fagron	Estriol	12A26-N02	2
Fagron	Estriol	12F08-N06	1
Fagron	Estriol	12H06-N02	5
Fagron	Estriol	12H06-No2	2
Fagron	Estriol	12K07-N15	2
Fagron	Estriol	13C15-N04	4
Fagron	Estriol	13D19-N02	1
Fagron	Estriol	13H28-N01	4
Fagron	Estriol	14B06-B11-291563	1
Fagron	Estriol	14b06b11291565	1
Fagron	Estriol	14B06-B11-291565	1
Fagron	Estriol	14B06-B11-294565	1
Fagron	Estriol	14E13-B01-294033	1
Fagron	Estriol	14E13-B01-294034	3
Fagron	Estriol	15297804	2
Fagron	Estriol	15A15-B07-312064	2
Fagron	Estriol	15A15-B07-314241	2
Fagron	Estriol	16/19-B01-332862	1
Fagron	Estriol	16/19-B01-336394	1
Fagron	Estriol	16/19-B01-340536	3
Fagron	Estriol	16/19-B01-3430535	1
Fagron	Estriol	16/19-B01-348555	1
Fagron	Estriol	16/19-B01-351346	3
Fagron	Estriol	1619B01351346	1
Fagron	Estriol	1629-b01-3363964	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Estriol	16D15-B03-323016	2
Fagron	Estriol	16D15-B03-323017	1
Fagron	Estriol	16I19-B01	2
Fagron	Estriol	16I19-B01-331466	1
Fagron	Estriol	16I19-B01-331467	1
Fagron	Estriol	16I19-B01-331468	1
Fagron	Estriol	16I19-B01-332862	1
Fagron	Estriol	16I19-B01-340535	2
Fagron	Estriol	16I19-B01-348555	1
Fagron	Estriol	16I19-B01-351346	1
Fagron	Estriol	16I9-B01	1
Fagron	Estriol	19C28-B01	1
Fagron	Estriol	19C28-B01-361787	3
Fagron	Estriol	19C28-B01-361788	1
Fagron	Estriol	20F16-F02	1
Fagron	Estriol	20F16-F02-372831	1
Fagron	Estriol	20f16-f02-372833	1
Fagron	Estriol	20G10-F06	7
Fagron	Estriol	20G10-F06-3729304	1
Fagron	Estriol	20G10-F06-372933	1
Fagron	Estriol	20g10-f06-372934	1
Fagron	Estriol	20g10-F06-372934	1
Fagron	Estriol	20G10-F06-372934	15
Fagron	Estriol	20G10-F06-372936	1
Fagron	Estriol	20G10-F06372958	1
Fagron	Estriol	20G10-F06-372958	28
Fagron	Estriol	20G10-F06-379234	1
Fagron	Estriol	20G10-FO6-372935	1
Fagron	Estriol	20G10-FO6-372958	1
Fagron	Estriol	21B26-F01	1
Fagron	Estriol	21B26-F01-378475	1
Fagron	Estriol	21B26-F01-379597	1
Fagron	Estriol	21B26-F01-380778	1
Fagron	Estriol	22A10-F03-381434	2
Fagron	Estriol	22A10-F03-381730	1
Fagron	Estriol	22H12-B05-224456	1
Fagron	Estriol	22H12-B06	1
Fagron	Estriol	22H12-B06-222365	3
Fagron	Estriol	22H12-B06-222366	1
Fagron	Estriol	22H12-BO6-222366	1
Fagron	Estriol	23A30-B01-227262	1
Fagron	Estriol	23H03-B06-233745	1
Fagron	Estriol	2OG10-F06-372934	1
Fagron	Estriol	2OG10-FO6-372934	1
Fagron	Estriol	700194-0001	1
Fagron	Estriol	81100490	1
Fagron	Estriol	86200800	3
Fagron	Estriol	F02-3728302	1
Fagron	Estriol	F06_3729508	1
Fagron	Estriol	F06-3729303	1
Fagron	Estriol	F06-3729304	3
Fagron	Estriol	F06-372933	1
Fagron	Estriol	F06-3729508	3
Fagron	Estriol	L00047276	11
fargon	Estriol	12a26-n02	1
Fiebig	Estriol	17133711	2
Fischar/Gehe	Estriol	14H29-B02-298072	3
Gehe 30.12.14	Estriol	14B06-B11-291563	1
Gehe	Estriol	16053405	1
Gehe	Estriol	17348701	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Estriol	17133706	1
Geilenkirchen	Estriol	17133710	1
Geilenkirchen	Estriol	17348701	1
Haihang Industry	Estriol	20130824	1
Jenne	Estriol	F06-3729508	1
Kehr	Estriol	17133704	1
Kehr	Estriol	18247101	1
Noweda 19.05.2015	Estriol	14272104	1
Noweda	Estriol	11J13-No7	1
Noweda	Estriol	12032504	1
Noweda	Estriol	16I19-B01	1
Noweda	Estriol	19C28-B01-361786	1
Noweda	Estriol	20G10-F06	1
Noweda	Estriol	20G10-F06-372933	2
Noweda	Estriol	2103007	1
NWM CHina	Estriol	ES150304	1
Phoenix	Estriol	17348701	1
Phoenix	Estriol	20G10-F06-372958	1
Phoenix	Estriol	3032	1
Phönix /euro	Estriol	1803011-01	1
Phönix	Estriol	16/19-B01331467	1
Sanacorp	Estriol	13256004	1
Sanacorp	Estriol	16317701	1
Sanacorp	Estriol	16317702	1
Sanacorp	Estriol	19035606	1
sanacorp	Estriol	2103007-01	1
Sanacorp	Estriol	2111005-01	1
Shandong Northwest M...	Estriol	ETL160302	1
Shandong Northwest M...	Estriol	ETL160419	1
VDL	Estriol	13256004	1

- 235 439 spectra from 1515 *Apo-Ident* customers from a total of 49 058 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estriol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estriol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	855	0	152 107
Type B	0	1777	0	200 307
Type C	0	618	10	235 439

The substance/substance group *Estriol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2982 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6624 %)
Type C	100.0000 % (> 99.9007 %)	98.4076 % (> 97.9299 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20878	21255	5,90	179,06
21255	21255	0,00	177,90
21390	21390	0,00	196,83
21391	21390	5,03	197,39
21392	21939	5,34	194,64
21393	21848	5,67	196,31
21394	21939	4,82	193,04
21395	21848	2,43	198,69
21399	21939	2,91	174,98
21400	21939	4,60	178,71
21401	21390	3,59	199,38
21404	21939	3,20	168,17
21848	21848	0,00	198,84
21939	21939	0,00	178,08
22889	23181	3,03	150,27
23172	21939	3,78	159,36
23181	23181	0,00	152,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Etinilestradiol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20950-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Etinilestradiol; Ethinylestradiolum

Special notes

When selecting the *Etinilestradiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Etinilestradiol	6	2	19

Second-stage model

For differentiation of the substance/substance group *Etinilestradiol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Etinilestradiol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	108,98	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Etinilestradiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Etinilestradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Etinilestradiol	13I09-N04	20950	40	1402058
Fagron	Etinilestradiol	14E15-B03-296049	21705	55	1507109
Fagron	Etinilestradiol	14E15-B03-296049	21705SI	56	1507109
Fagron	Etinilestradiol	14E15-B03-310270	21916	60	20140708
Fagron	Etinilestradiol	14E15-B03-310270	21916SI	60	20140708
Fagron	Etinilestradiol	14E15-B03-310270	21958	60	20140708
Fagron	Etinilestradiol	18E25-B01-355721	24584	40	20180810
Fagron	Etinilestradiol	19J11-F01-367137	25045	40	2007191
Fagron	Etinilestradiol	22A18-F02-382202	26327	40	20220429
Fagron	Etinilestradiol	22A18-F02-382202	26327SI	40	20220429

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 491 spectra of 10 reference samples from the substance/substance group *Etinilestradiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

different batches.

- 152 471 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 312 spectra of 7 reference samples from the substance/substance group *Etinilestradiol*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Etinilestradiol	16B17-B01-329904	23075	40
Fagron	Etinilestradiol	23E16-B04-234620	27053	40
Fagron	Etinilestradiol	14E15-B03-310270	21958SI†	43
Fagron	Etinilestradiol	16B17-B01-329904	23075SI	30
Fagron	Etinilestradiol	18E25-B01-355721	24584SI†	40
Fagron	Etinilestradiol	19J11-F01-367137	25045SI†	40
Fagron	Etinilestradiol	23E16-B04-234620	27053SI	79

- 201 772 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 36 spectra from 28 *Apo-Ident* customers from 23 batches from the substance/substance group *Etinilestradiol*.

- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caelo	Etinilestradiol	18E25-B01-0001	1
Fagron	Etinilestradiol	12D19-N04	1
Fagron	Etinilestradiol	1367138	2
Fagron	Etinilestradiol	13G03-N04	1
Fagron	Etinilestradiol	13I09-N04	1
Fagron	Etinilestradiol	14e15b03296049	1
Fagron	Etinilestradiol	16B17-B01	1
Fagron	Etinilestradiol	16B17-B01-320666	1
Fagron	Etinilestradiol	16B17-B01-333326	1
Fagron	Etinilestradiol	18E25-B01	2
Fagron	Etinilestradiol	18E25-B01-351832	2
Fagron	Etinilestradiol	18E25-B01-352721	1
Fagron	Etinilestradiol	18E25-B01-353920	3
Fagron	Etinilestradiol	18E25-B01-355721	4
Fagron	Etinilestradiol	19J11-F01-367137	1
Fagron	Etinilestradiol	19J11-F01-367138	5
Fagron	Etinilestradiol	19J11-F01-373282	2
Fagron	Etinilestradiol	22A18-F02-382202	1
Fagron	Etinilestradiol	22A18-FO2-382202	1
Fagron	Etinilestradiol	84100720	1
Fagron	Etinilestradiol	8561175	1
Fagron	Etinilestradiol	F01-3671308	1
Fagron	Etinilestradiol	UN803HA	1

- 236 031 spectra from 1515 *Apo-Ident* customers from a total of 49 235 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Etinilestradiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Etinilestradiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	491	0	152 471
Type B	0	312	0	201 772
Type C	0	36	0	236 031

The substance/substance group *Etinilestradiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7780 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0769 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 83.3333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20950	20950	0,00	172,20
21705	21705	0,00	207,26
21916	21705	9,70	189,12
21958	21705	8,61	192,25
24584	20950	40,25	159,16
25045	25045	0,00	215,29
26327	20950	30,28	169,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Etossuximida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24100-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Etossuximida; Ethosuximidum

Special notes

When selecting the *Etossuximida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Etossuximida	2	1	0

Second-stage model

For differentiation of the substance/substance group *Etossuximida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Etossuximida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	73,65	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Etossuximida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Etossuximida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Katwijk Ch...	Etossuximida	451717	24100	40	20180509
Katwijk Ch...	Etossuximida	451645	24101	40	1807457

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Etossuximida*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Etossuximida*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Katwijk Chemie BV	Etossuximida	451644	24102	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Etossuximida*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Etossuximida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Etossuximida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Etossuximida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24100	24101	31,68	118,58
24101	24101	0,00	120,43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fampridina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20902-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fampridina; Fampridinum

Special notes

When selecting the *Fampridina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fampridina	9	5	46

Second-stage model

For differentiation of the substance/substance group *Fampridina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fampridina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	153,67	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fampridina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fampridina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fampridina	16276001	22881	40	20161024
Caelo	Fampridina	16276001	22905	40	20161024
Caelo	Fampridina	16276001	23074	40	20161024
Caelo	Fampridina	16276001	23237	40	20161024
Caelo	Fampridina	190675	24724	40	20190506*
Caelo	Fampridina	180219	24756	40	20180214*
Caelo	Fampridina	180219	24756SI	40	20180214*
Caelo	Fampridina	20003524	25559	40	20201126*
Caelo	Fampridina	20003524	25559SI	40	20201126*
Fagron	Fampridina	13G26-N06	20902	40	1402686
Fagron	Fampridina	14D11-B06-293750	21541	60	20140113
Fagron	Fampridina	16D11-B07-318220	22491	40	AR-16-FG-011566-01
Fagron	Fampridina	16E25-B03-324097	22894	40	20160609
Fagron	Fampridina	16E25-B03-324097	22945	40	20160609
Fagron	Fampridina	17K20-B02-349165	24439	40	20180103
Fagron	Fampridina	17K20-B02-349165	24439SI	40	20180103

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 660 spectra of 16 reference samples from the substance/substance group *Fampridina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 302 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 435 spectra of 11 reference samples from the substance/substance group *Fampridina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fampridina	172170	23653	40
Caelo	Fampridina	19000755	25197	40
Caelo	Fampridina	22001045	26119	40
Fagron	Fampridina	19G24-B02-363769	24823	40
Fagron	Fampridina	22I21-B07-223809	26385	40
Caelo	Fampridina	190675	24724SI†	40
Caelo	Fampridina	19000755	25197SI	40
Caelo	Fampridina	22001045	26119SI	40
Fagron	Fampridina	16E25-B03-324097	22894SI†	40
Fagron	Fampridina	19G24-B02-363769	24823SI	35
Fagron	Fampridina	22I21-B07-223809	26385SI	40

- 201 649 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 79 spectra from 24 *Apo-Ident* customers from 48 batches from the substance/substance group *Fampridina*.
- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fampridina	22K17-B03-228705	1
	Fampridina	353033	1
Caelo	Fampridina	15350001	1
Caelo	Fampridina	15350002	1
Caelo	Fampridina	16276001	1
Caelo	Fampridina	16276002	3
Caelo	Fampridina	17217002	1
Caelo	Fampridina	17217003	2
Caelo	Fampridina	17217004	1
Caelo	Fampridina	17217005	1
Caelo	Fampridina	18021901	1
Caelo	Fampridina	18021903	2
Caelo	Fampridina	18021907	3
Caelo	Fampridina	19000755005	2
Caelo	Fampridina	19000755007	1
Caelo	Fampridina	19067501	1
Caelo	Fampridina	19067504	1
Caelo	Fampridina	24111801	1
Caesar & Loretz GmbH/Gehe	Fampridina	22001045001	2
Fagron	Fampridina	13C07-B02-289395	1
Fagron	Fampridina	14D11-B06-296110	1
Fagron	Fampridina	14D11-B40-301641	1
Fagron	Fampridina	14D11-B40-304961	1
Fagron	Fampridina	16/19-Bo4-330727	1
Fagron	Fampridina	16D11-B07	1
Fagron	Fampridina	17/19-B01	2
Fagron	Fampridina	17/19-B01-339467	1
Fagron	Fampridina	17D19-B01-333745	1
Fagron	Fampridina	17K20_B02_344609	1
Fagron	Fampridina	17K20-B02	4
Fagron	Fampridina	17K20-B02-344609	2
Fagron	Fampridina	17K20-B02-349165	1
Fagron	Fampridina	17K20-B02-349165/0000254876	1
Fagron	Fampridina	18121801	1
Fagron	Fampridina	18H01-B08	1
Fagron	Fampridina	19G24-B02	4
Fagron	Fampridina	19G24-B02-363768	5
Fagron	Fampridina	19g24-b02-363769	1
Fagron	Fampridina	19G24-B02-363770	9
Fagron	Fampridina	20D06-F07-370084	2
Fagron	Fampridina	20D06-F07-370086	2
Fagron	Fampridina	22C25-B07-215458	1
Fagron	Fampridina	22C25-B07-215459	1
Fagron	Fampridina	22k17-b03-226121	1
Fagron	Fampridina	254876	1
Inresa	Fampridina	220825	1
Inresa	Fampridina	236761	1
Noweda	Fampridina	17K20-B02-349165	1
PHÖNIX	Fampridina	20210217-2	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 988 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fampridina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fampridina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	660	0	152 302
Type B	0	435	0	201 649
Type C	0	78	1	235 988

The substance/substance group *Fampridina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0909 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6207 %)
Type C	100.0000 % (> 99.9007 %)	98.7342 % (> 94.9367 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20902	20902	0,00	268,63
21541	20902	7,36	271,04
22491	22491	0,00	293,16
22881	20902	33,50	271,48
22894	22491	7,58	290,23
22905	20902	31,26	272,02
22945	22491	12,03	288,27
23074	20902	35,25	271,18
23237	22491	36,60	271,82
24439	22491	7,95	293,36

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24724	24724	0,00	266,49
24756	24756	0,00	267,37
25559	25559	0,00	255,62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fenazona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22532-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fenazona; Phenazonum

Special notes

When selecting the *Fenazona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fenazona	7	4	4

Second-stage model

For differentiation of the substance/substance group *Fenazona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fenazona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	99,95	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fenazona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fenazona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fenazona	15415101	22576	40	20151215
Caelo	Fenazona	15415107	22827	40	20151215
Caelo	Fenazona	181347	24259	40	20180629*
Fagron	Fenazona	13G16-B07-287172	22532	40	AR-16-FG-011360-01
Fagron	Fenazona	13G16-B07-287172	22720	40	20130814
Fagron	Fenazona	15H28-B09-322944	24698	40	20150916
Fagron	Fenazona	21B23-B97-210607	25589	40	20210301
Fagron	Fenazona	22K28-B11-226183	26468	40	20221214
Fagron	Fenazona	22K28-B11-226183	26468SI	20	20221214

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 340 spectra of 9 reference samples from the substance/substance group *Fenazona*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 4 reference samples from the substance/substance group *Fenazona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fenazona	170836	23302	40
Caelo	Fenazona	182565	24369	40
Caelo	Fenazona	21002059	25797	50
Caelo	Fenazona	21003237	25847	50

- 201 904 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Fenazona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Fenazona	17083601	1
Caelo	Fenazona	18061101	1
Caelo	Fenazona	181347001	1
Caelo	Fenazona	182565002	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fenazona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fenazona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	180	0	201 904
Type C	0	4	0	236 063

The substance/substance group *Fenazona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22532	22532	0,00	199,58
22576	22532	10,93	198,97
22720	22532	3,10	200,93
22827	22532	9,09	199,00
24259	24259	0,00	196,72
24698	22532	17,72	200,48
25589	22532	16,61	202,44
26468	22532	15,96	207,63

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fenilbutazona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20447-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fenilbutazona; Phenylbutazonum

Special notes

When selecting the *Fenilbutazona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fenilbutazona	8	5	12

Second-stage model

For differentiation of the substance/substance group *Fenilbutazona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fenilbutazona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	126,01	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fenilbutazona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fenilbutazona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fenilbutazona	14057202	21379	40	20140321
Caelo	Fenilbutazona	161121	22471	60	20160331*
Euro OTC	Fenilbutazona	1305050-02	21605	60	AR-15-FG-005687-01
Euro OTC	Fenilbutazona	1507023	21855	60	20150805*
Euro OTC	Fenilbutazona	1908013	24861	40	20190923*
Euro OTC	Fenilbutazona	2001046	25239	40	20200728*
Euro OTC	Fenilbutazona	2101032	25535	40	20210218*
Euro OTC	Fenilbutazona	2209001	26347	40	20220921*
Euro OTC	Fenilbutazona	2209001	26347SI	20	20220921*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Fenilbutazona*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 6 reference samples from the substance/substance group *Fenilbutazona*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Fenilbutazona	1604033	22563	40
Euro OTC	Fenilbutazona	1804018	24122	40
Euro OTC	Fenilbutazona	2107012	25830	50
Fagron	Fenilbutazona	18B21-B06-361114	24952	40
Fagron	Fenilbutazona	22G22-B03-221076	26451	40
Euro OTC	Fenilbutazona	2107012	25830SI	10

- 201 864 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 11 *Apo-Ident* customers from 12 batches from the substance/substance group *Fenilbutazona*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Fenilbutazona	10262901	1
Caelo	Fenilbutazona	14099511	1
Caelo	Fenilbutazona	15218502	1
Caelo	Fenilbutazona	18063205	1
Euro OTC	Fenilbutazona	130505_01	1
Euro OTC	Fenilbutazona	170612PB/1604033-01	1
Euro OTC	Fenilbutazona	180401802	1
Euro OTC	Fenilbutazona	1804018-03	1
Euro OTC	Fenilbutazona	19091806	1
Euro OTC	Fenilbutazona	2001046-01	1
Fagron	Fenilbutazona	11H26-N02	1
Fagron	Fenilbutazona	13D30-N16	1

- 236 055 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fenilbutazona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fenilbutazona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	220	0	201 864
Type C	0	12	0	236 055

The substance/substance group *Fenilbutazona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21379	21605	5,19	217,82
21605	21605	0,00	212,75
21855	21855	0,00	216,16
22471	22471	0,00	214,78
24861	24861	0,00	222,53
25239	25239	0,00	222,13
25535	25535	0,00	224,70
26347	26347	0,00	224,54

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fenitoína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20949-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fenitoína; Phenytoinum

Special notes

When selecting the *Fenitoína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fenitoína	5	3	3

Second-stage model

For differentiation of the substance/substance group *Fenitoína* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fenitoína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	106,70	–
⋮	⋮	⋮
Sacarina sódica	>50	86,00
Cloridrato de propranolol	>50	113,41
Quinolina amarela	>50	139,79
Sulfato de atropina	>50	165,12
Furoato de mometasona	>50	191,45
Citrato monobásico de magnésio, hid…	>50	254,17
Orotato de cálcio di-hidratado	>50	262,23
Sorbato de potássio	>50	371,26
Hidrocortisona	>50	398,03
Escina, hidrossolúvel	>50	643,74

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fenitoína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fenitoína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Fenitoína	13G26-N02	20949	40	1401380
Fagron	Fenitoína	15E12-B05-312661	22271	45	20150519
Fagron	Fenitoína	18F01-B02-350492	24438	40	20180705
Fagron	Fenitoína	18F01-B02-350492	24693	40	20180705
Fagron	Fenitoína	19E14-B02	24818	40	20190722
Fagron	Fenitoína	22A17-F03-381312	27041	40	20220301

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 245 spectra of 6 reference samples from the substance/substance group *Fenitoína*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 717 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Fenitoína*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Fenitoína	12I07-N02	20678	40
Fagron	Fenitoína	16C14-B06-325086	23110	40
Fagron	Fenitoína	17L22-B04-345861	23994	40
Fagron	Fenitoína	16C14-B06-325086	23377	40
Fagron	Fenitoína	22A17-F03-381312	27041SI†	20

- 201 904 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Fenitoína*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fenitoína	22A17-F03-381312	1
Caelo	Fenitoína	17L22-B04-345861	1
Fagron	Fenitoína	12C27N13	1
Fagron	Fenitoína	12I07-N02	1
Fagron	Fenitoína	13G26-N02	1
Fagron	Fenitoína	22A17-F03-381312	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fenitoína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fenitoína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	245	0	152 717
Type B	0	180	0	201 904
Type C	0	6	0	236 061

The substance/substance group *Fenitoína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5510 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20949	20949	0,00	316,53
22271	20949	18,03	316,71
24438	20949	7,96	316,10
24693	20949	5,49	317,74
24818	20949	7,07	316,55
27041	20949	24,64	309,94

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fenobarbital**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20311-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fenobarbital; Phenobarbitalum

Special notes

When selecting the *Fenobarbital* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fenobarbital	4	1	18

Second-stage model

For differentiation of the substance/substance group *Fenobarbital* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fenobarbital* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citrato de cafeína	131,11	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fenobarbital* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fenobarbital*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fenobarbital	12173202	21198	40	0914E-01040
Caelo	Fenobarbital	12173202	21198SI	60	0914E-01040
Fagron	Fenobarbital	15G07-B06-311718	22420	60	1416Q-01040
Fagron	Fenobarbital	15G07-B06-311718	22420SI	60	1416Q-01040
Th. Geyer	Fenobarbital	67045	21200	40	0914F-01040
Th. Geyer	Fenobarbital	67045	21200SI	60	0914F-01040
Th. Geyer	Fenobarbital	067056	23497	40	2017A-01040

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 7 reference samples from the substance/substance group *Fenobarbital*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 602 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Fenobarbital*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Fenobarbital	16G20-B04-328344	23496	40
Fagron	Fenobarbital	16G20-B04-328344	23496SI	40
Th. Geyer	Fenobarbital	067056	23497SI†	40

- 201 964 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 57 spectra from 28 *Apo-Ident* customers from 20 batches from the substance/substance group *Fenobarbital*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fenobarbital	21A19-F02	2
	Fenobarbital	21A19-F02-376671	2
	Fenobarbital	22D19-F03-384178	2
	Fenobarbital	70510	1
AHD	Fenobarbital	67045	1
BLS	Fenobarbital	67056	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Fenobarbital	13G05-N09	1
Fagron	Fenobarbital	15G07-B06-311718	1
Fagron	Fenobarbital	15I18-B08-318544	1
Fagron	Fenobarbital	16G20-B04-328344	3
Fagron	Fenobarbital	18C07-B01-347288	4
Fagron	Fenobarbital	18H15-B01-354934	2
Fagron	Fenobarbital	19G23-B01	1
Fagron	Fenobarbital	19G23-B01-363364	1
Fagron	Fenobarbital	19G23-B01-363958	1
Fagron	Fenobarbital	19G23-B01-365593	3
Fagron	Fenobarbital	21A19-F02	1
Fagron	Fenobarbital	21A19-F02-376671	3
Fagron	Fenobarbital	B01-3549304	1
Fagron	Fenobarbital	B01-3639508	1
Fagron	Fenobarbital	B01-3655903	1
Fagron	Fenobarbital	F02-3766701	1
Gehe	Fenobarbital	70510	1
Th. Geyer	Fenobarbital	67045	2
Th. Geyer	Fenobarbital	67056	4
Th. Geyer	Fenobarbital	70510	15

- 236 010 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fenobarbital* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fenobarbital* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	120	0	201 964
Type C	0	54	3	236 010

The substance/substance group *Fenobarbital* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	94.7368 % (> 89.4737 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21198	21198	0,00	319,01
21200	21200	0,00	321,39
22420	22420	0,00	321,90
23497	23497	0,00	321,40

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Finasterida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20955-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Finasterida; Finasteridum

Special notes

When selecting the *Finasterida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Finasterida	7	13	33

Second-stage model

For differentiation of the substance/substance group *Finasterida* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Finasterida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	106,92	135,77
⋮	⋮	⋮
Fosfato sódico de riboflavina hidratado	>50	163,56
Fosfato de Mg-Ca-K-colamina	>50	360,86
Citrato de magnésio	>50	361,34
Sulfato de gentamicina	>50	786,20
Sulfato de tobramicina	>50	969,08
Sulfato de neomicina	>50	1163,29
Gluconato de zinco	>50	1660,09
Tetraborato de sódio	>50	2082,92

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Finasterida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Finasterida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Finasterida	1403016-01	21626	60	1506004
Euro OTC	Finasterida	1403016-02	21750	60	20140505
Euro OTC	Finasterida	1403016-02	21750SI	51	20140505
Euro OTC	Finasterida	1605020	22565	40	20160613*
Euro OTC	Finasterida	1605020	22565SI	40	20160613*
Euro OTC	Finasterida	1610012	22856	40	20161116*
Euro OTC	Finasterida	1610012	22856SI	33	20161116*
Euro OTC	Finasterida	2101024	25527	40	20210217*
Euro OTC	Finasterida	2101024	25527SI	34	20210217*
Fagron	Finasterida	13I03-N01	20955	40	1411272
Fagron	Finasterida	14A16-B40-295980	21742	60	20140317
Fagron	Finasterida	14A16-B40-295980	21742SI	45	20140317

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 543 spectra of 12 reference samples from the substance/substance group *Finasterida*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 419 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1052 spectra of 27 reference samples from the substance/substance group *Finasterida*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Finasterida	1704004	23151	40
Euro OTC	Finasterida	1804010	24129	40
Euro OTC	Finasterida	1809019	24342	40
Euro OTC	Finasterida	2003027	25355	40
Euro OTC	Finasterida	2111004	25913	40
Euro OTC	Finasterida	2210013	26421	40
Euro OTC	Finasterida	2210015	26438	40
Euro OTC	Finasterida	2301045	26576	40
Euro OTC	Finasterida	2403004	27291	40
Euro OTC	Finasterida	2407022	27367	30
Fagron	Finasterida	15J15-B02-320084	22594	40
Fagron	Finasterida	22B14-B09-217630	26078	40
Fagron	Finasterida	23J19-B04-233067	27039	40
Euro OTC	Finasterida	1804010	24129SI	40
Euro OTC	Finasterida	1809019	24342SI	31
Euro OTC	Finasterida	2003027	25355SI	39
Euro OTC	Finasterida	2111004	25913SI	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Finasterida	2210013	26421SI	40
Euro OTC	Finasterida	2210015	26438SI	40
Euro OTC	Finasterida	2301045	26576SI	40
Euro OTC	Finasterida	2403004	27291SI	40
Euro OTC	Finasterida	2407022	27367SI	38
Fagron	Finasterida	15J15-B02-320084	22594SI	40
Fagron	Finasterida	15J15-B02-320084	22595	40
Fagron	Finasterida	15J15-B02-320084	22595SI	40
Fagron	Finasterida	22B14-B09-217630	26078SI	40
Fagron	Finasterida	23J19-B04-233067	27039SI	34

- 201 032 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 53 spectra from 19 *Apo-Ident* customers from 35 batches from the substance/substance group *Finasterida*.

- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Finasterida	17I12-B07-340606	1
Caelo	Finasterida	1809019-01	1
Crystal	Finasterida	141100801	1
Euro OTC	Finasterida	1403016-02	1
Euro OTC	Finasterida	1411008-01	1
Euro OTC	Finasterida	1605020-01	1
Euro OTC	Finasterida	1610012-01	2
Euro OTC	Finasterida	1704004-01	5
Euro OTC	Finasterida	1804010-01	2
Euro OTC	Finasterida	1809019-01	2
Euro OTC	Finasterida	18090919-01	1
Euro OTC	Finasterida	20B11-F03-373005	1
Euro OTC	Finasterida	2101024-01	1
Euro OTC	Finasterida	2210013-01	1
Euro OTC	Finasterida	C1012/116010	1
Fagron	Finasterida	13I03-N01	2
Fagron	Finasterida	14111305	1
Fagron	Finasterida	14L23-B02-306981	1
Fagron	Finasterida	15I01-B03	1
Fagron	Finasterida	15I01-B03-314476	1
Fagron	Finasterida	17011303	1
Fagron	Finasterida	17I12-B07-340606	4
Fagron	Finasterida	17I12-B07-355068	1
Fagron	Finasterida	17I12-B07-356321	1
Fagron	Finasterida	18041810	1
Fagron	Finasterida	18L13-B05-356320	1
Fagron	Finasterida	18L13-B05-356321	2
Fagron	Finasterida	19041707	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Finasterida	19D10-B01-362337	3
Fagron	Finasterida	20181101	1
Fagron	Finasterida	20190301	1
Fagron	Finasterida	20190702	1
Fagron	Finasterida	20B11-F03-373005	1
Fagron	Finasterida	20J01-F05-374980	1
Fagron	Finasterida	22B14-B09-217630	2
Fagron	Finasterida	F03-3730005	1
Phoenix	Finasterida	1804010-01	1
Shandong Northwest M...	Finasterida	FNA160604	1

- 236 014 spectra from 1515 *Apo-Ident* customers from a total of 49 223 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Finasterida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Finasterida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	543	0	152 419
Type B	0	1052	0	201 032
Type C	0	53	0	236 014

The substance/substance group *Finasterida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8950 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4297 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 88.6792 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20955	20955	0,00	187,42
21626	21626	0,00	179,27
21742	21626	24,73	178,64
21750	21626	20,63	177,74
22565	22565	0,00	182,69
22856	22856	0,00	185,55
25527	25527	0,00	188,58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fluocinolona acetonida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21031-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fluocinolona acetonida; Fluocinoloni acetonidum

Special notes

When selecting the *Fluocinolona acetonida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fluocinolona acetonida	6	3	43

Second-stage model

For differentiation of the substance/substance group *Fluocinolona acetonida* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fluocinolona acetonida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Triancinolona acetonido	59,79	36,51
⋮	⋮	⋮
Betametasona	>50	65,70
Dexametasona	>50	73,91
Metilprednisolona	>50	82,43
Tirotricina	>50	87,41
Prednisolona	>50	87,53
Gramicidina	>50	153,42

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fluocinolona acetonida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fluocinolona acetonida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fluocinolona acetonida	12035003	21756	60	20120321
Caelo	Fluocinolona acetonida	12035003	21756SI	48	20120321
Caelo	Fluocinolona acetonida	162281	22637	40	20160907*
Caelo	Fluocinolona acetonida	162281	22637SI	30	20160907*
Euro OTC	Fluocinolona acetonida	2804013E-01	21031	60	1404008
Euro OTC	Fluocinolona acetonida	2804013E-01	21077	60	20121206
Euro OTC	Fluocinolona acetonida	2804013E-01	21822	60	20121206
Euro OTC	Fluocinolona acetonida	2804013E-01	21822SI	60	20121206
Fagron	Fluocinolona acetonida	14L19-B04-307101	22267	45	20150219
Fagron	Fluocinolona acetonida	14L19-B04-307101	22267SI	45	20150219
Fagron	Fluocinolona acetonida	14L19-B04-307101	23080	40	20150219
Fagron	Fluocinolona acetonida	17F14-B08-350105	24700	40	20171221
Fagron	Fluocinolona acetonida	20K03-F03-375403	25750	40	2111539
Fagron	Fluocinolona acetonida	20K03-F03-375403	25750SI	40	2111539

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 668 spectra of 14 reference samples from the substance/substance group *Fluocinolona acetonida*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 294 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 378 spectra of 10 reference samples from the substance/substance group *Fluocinolona acetonida*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fluocinolona acetonida	172130	23674	40
Fagron	Fluocinolona acetonida	21K03-B06-217656	26069	40
Fagron	Fluocinolona acetonida	22D11-B02-221847	26325	40
Caelo	Fluocinolona acetonida	172130	23674SI	12
Euro OTC	Fluocinolona acetonida	2804013E-01	21823	60
Euro OTC	Fluocinolona acetonida	2804013E-01	21823SI	46
Fagron	Fluocinolona acetonida	14L19-B04-307101	23080SI†	20
Fagron	Fluocinolona acetonida	17F14-B08-350105	24700SI†	40
Fagron	Fluocinolona acetonida	21K03-B06-217656	26069SI	40
Fagron	Fluocinolona acetonida	22D11-B02-221847	26325SI	40

- 201 706 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 66 spectra from 42 *Apo-Ident* customers from 48 batches from the substance/substance group *Fluocinolona acetonida*.
- Among them are spectra of independent samples from 43 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fluocinolona acetonida	22D11-B02-221848	1
	Fluocinolona acetonida	22D11-B02-221848	1
Caelo	Fluocinolona acetonida	12035003	1
Caelo	Fluocinolona acetonida	16228108	2
Caelo	Fluocinolona acetonida	18073203	1
Caelo	Fluocinolona acetonida	18073206	1
Caelo	Fluocinolona acetonida	18073303	2
Caelo	Fluocinolona acetonida	2804013V-03	1
Caesar & Loretz Hilden	Fluocinolona acetonida	18073301	1
Eurho	Fluocinolona acetonida	1408022-04	1
Euro OTC	Fluocinolona acetonida	1408022-02	4
Euro OTC	Fluocinolona acetonida	1408022-03	1
Euro OTC	Fluocinolona acetonida	2804013E-01	1
Fagro/Noweda	Fluocinolona acetonida	15K06-B02-336730	1
Fagron	Fluocinolona acetonida	1(18I19-B05-363303)	1
Fagron	Fluocinolona acetonida	13E22-N10	1
Fagron	Fluocinolona acetonida	13L30B35295489	1
Fagron	Fluocinolona acetonida	13L30-B35-295489	1
Fagron	Fluocinolona acetonida	14l19-b04	1
Fagron	Fluocinolona acetonida	14L19-B04	4
Fagron	Fluocinolona acetonida	14L19-B04-317248	2
Fagron	Fluocinolona acetonida	14L19-B04-615699	1
Fagron	Fluocinolona acetonida	15K06-B02	1
Fagron	Fluocinolona acetonida	15k06-b02-326488	1
Fagron	Fluocinolona acetonida	15k06-b02-332955	1
Fagron	Fluocinolona acetonida	15K06-B02-336730	1
Fagron	Fluocinolona acetonida	17f14-b08-346965	1
Fagron	Fluocinolona acetonida	17F14-B08-346965	1
Fagron	Fluocinolona acetonida	17F14-B08-350106	3
Fagron	Fluocinolona acetonida	18/19-B05-359031	1
Fagron	Fluocinolona acetonida	18/19-B05-365691	1
Fagron	Fluocinolona acetonida	18/19-B05-370559	1
Fagron	Fluocinolona acetonida	18I19B05-358085	1
Fagron	Fluocinolona acetonida	18I19-B05-358085	2
Fagron	Fluocinolona acetonida	18I19-B05-363303	1
Fagron	Fluocinolona acetonida	18I19-B05-365691	1
Fagron	Fluocinolona acetonida	2151nm1b0091723	1
Fagron	Fluocinolona acetonida	2151NM1B0091723	2
Fagron	Fluocinolona acetonida	21H13-B18-213858	2
Fagron	Fluocinolona acetonida	21K03-B06	2
Fagron	Fluocinolona acetonida	22D11-B02-221848	1
Fagron	Fluocinolona acetonida	B05-3590301	1
Fagron	Fluocinolona acetonida	B05-3633003	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Fluocinolona acetonida	B05-3705509	1
Fargon/Kehr	Fluocinolona acetonida	14L-19-B04	1
Fargon/Noweda	Fluocinolona acetonida	13L13-B35	1
Farmabios s.p.A	Fluocinolona acetonida	C24H30F206	1
Gehe	Fluocinolona acetonida	18/19-B05	1
Ichthyol Gesellschaf…	Fluocinolona acetonida	14L19-B04-321003	1
Kehr	Fluocinolona acetonida	17F14-B08-346965	1
Noweda	Fluocinolona acetonida	23D01-B03-231001	1

- 236 001 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fluocinolona acetonida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fluocinolona acetonida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	668	0	152 294
Type B	0	378	0	201 706
Type C	0	66	0	236 001

The substance/substance group *Fluocinolona acetonida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1018 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4127 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.9091 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21031	21031	0,00	63,04
21077	21031	4,38	63,96
21756	21031	22,59	62,97
21822	21031	19,63	64,63
22267	21031	17,79	62,87
22637	22637	0,00	119,13
23080	21031	20,38	59,79
24700	21031	11,30	60,27
25750	25750	0,00	113,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fosfato de cálcio monobásico di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20129-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fosfato de cálcio monobásico di-hidratado; Calcii hydrogenphosphas dihydricus

Special notes

When selecting the *Fosfato de cálcio monobásico di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fosfato de cálcio monobásico di-hidratado	2	1	21

Second-stage model

For differentiation of the substance/substance group *Fosfato de cálcio monobásico di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fosfato de cálcio monobásico di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	58,83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fosfato de cálcio monobásico di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fosfato de cálcio monobásico di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fosfato de cálcio monobás…	181117	24225	40	20180528*
Caelo	Fosfato de cálcio monobás…	22001222	26566	40	20220607*
Caelo	Fosfato de cálcio monobás…	22001222	26566SI	20	20220607*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Fosfato de cálcio monobásico di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 862 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Fosfato de cálcio monobásico di-hidratado*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fosfato de cálcio monobás…	23002987	27080	40
Caelo	Fosfato de cálcio monobás…	23002987	27080SI	20

- 202 024 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 26 *Apo-Ident* customers from 21 batches from the substance/substance group *Fosfato de cálcio monobásico di-hidratado*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Fosfato de cálcio monobás…	101352009	1
Caelo	Fosfato de cálcio monobás…	10135201	1
Caelo	Fosfato de cálcio monobás…	10135216	1
Caelo	Fosfato de cálcio monobás…	10135223	1
Caelo	Fosfato de cálcio monobás…	10135228	1
Caelo	Fosfato de cálcio monobás…	11287501	1
Caelo	Fosfato de cálcio monobás…	11287503	2
Caelo	Fosfato de cálcio monobás…	11287509	2
Caelo	Fosfato de cálcio monobás…	11287510	1
Caelo	Fosfato de cálcio monobás…	12212804	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fosfato de cálcio monobás…	12212806	1
Caelo	Fosfato de cálcio monobás…	12212807	1
Caelo	Fosfato de cálcio monobás…	12212811	4
Caelo	Fosfato de cálcio monobás…	12212812	2
Caelo	Fosfato de cálcio monobás…	12212813	1
Caelo	Fosfato de cálcio monobás…	12212816	1
Caelo	Fosfato de cálcio monobás…	12212822	1
Caelo	Fosfato de cálcio monobás…	13170701	6
Caelo	Fosfato de cálcio monobás…	13170704	1
Caelo	Fosfato de cálcio monobás…	14011401	1
Caelo	Fosfato de cálcio monobás…	14085301	1
Cealo	Fosfato de cálcio monobás…	12212811	1
Phönix 12.12.2013	Fosfato de cálcio monobás…	13170704	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 237 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fosfato de cálcio monobásico di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fosfato de cálcio monobásico di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	60	0	202 024
Type C	0	33	5	236 029

The substance/substance group *Fosfato de cálcio monobásico di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9007 %)	86.8421 % (> 78.9474 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24225	24225	0,00	107,87
26566	26566	0,00	107,25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fosfato de codeína hemi-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20302-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fosfato de codeína hemi-hidratado; Codeini phosphas hemihydricus

Special notes

When selecting the *Fosfato de codeína hemi-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fosfato de codeína hemi-hidratado	7	3	44

Second-stage model

For differentiation of the substance/substance group *Fosfato de codeína hemi-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fosfato de codeína hemi-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	99,43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fosfato de codeína hemi-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fosfato de codeína hemi-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fosfato de codeína hemi-h…	13071504	21152	40	0814J-01279
Caelo	Fosfato de codeína hemi-h…	13071504	21152SI	60	0814J-01279
Caelo	Fosfato de codeína hemi-h…	15350703	22407	60	1316R-01279
Caelo	Fosfato de codeína hemi-h…	15350703	22407SI	60	1316R-01279
Fagron	Fosfato de codeína hemi-h…	13C11-N10	21148	40	0814I-01279
Fagron	Fosfato de codeína hemi-h…	13C11-N10	21148SI	60	0814I-01279
Fagron	Fosfato de codeína hemi-h…	15F09-B02-310520	22425	60	1316Q-01279
Fagron	Fosfato de codeína hemi-h…	15F09-B02-310520	22425SI	60	1316Q-01279
Fagron	Fosfato de codeína hemi-h…	16E17-B05-324109	23469	40	2017A-01279
Th. Geyer	Fosfato de codeína hemi-h…	67038	21150	40	0814K-01279
Th. Geyer	Fosfato de codeína hemi-h…	67038	21150SI	60	0814K-01279
Th. Geyer	Fosfato de codeína hemi-h…	067054	23466	40	2017D-01279

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 620 spectra of 12 reference samples from the substance/substance group *Fosfato de codeína hemi-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 342 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 8 reference samples from the substance/substance group *Fosfato de codeína hemi-hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fosfato de codeína hemi-h…	16349702	23467	40
Caelo	Fosfato de codeína hemi-h…	16169807	23468	40
Caelo	Fosfato de codeína hemi-h…	18187906	24650	40
Caelo	Fosfato de codeína hemi-h…	16349702	23467SI	40
Caelo	Fosfato de codeína hemi-h…	16169807	23468SI	40
Caelo	Fosfato de codeína hemi-h…	18187906	24650SI	40
Fagron	Fosfato de codeína hemi-h…	16E17-B05-324109	23469SI†	40
Th. Geyer	Fosfato de codeína hemi-h…	067054	23466SI†	40

- 201 764 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 135 spectra from 33 *Apo-Ident* customers from 49 batches from the substance/substance group *Fosfato de codeína hemi-hidratado*.

- Among them are spectra of independent samples from 44 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caeleo/ Kehr	Fosfato de codeína hemi-h…	181879001	2
Caelo	Fosfato de codeína hemi-h…	130715	1
Caelo	Fosfato de codeína hemi-h…	13I27-N06	1
Caelo	Fosfato de codeína hemi-h…	14275910	1
Caelo	Fosfato de codeína hemi-h…	1427910	1
Caelo	Fosfato de codeína hemi-h…	15219805	2
Caelo	Fosfato de codeína hemi-h…	15350703	2
Caelo	Fosfato de codeína hemi-h…	15350710	2
Caelo	Fosfato de codeína hemi-h…	16169805	3
Caelo	Fosfato de codeína hemi-h…	16349704	2
Caelo	Fosfato de codeína hemi-h…	16349706	2
Caelo	Fosfato de codeína hemi-h…	16349707	1
Caelo	Fosfato de codeína hemi-h…	16349708	2
Caelo	Fosfato de codeína hemi-h…	17160503	3
Caelo	Fosfato de codeína hemi-h…	17L22-B03-343752	1
Caelo	Fosfato de codeína hemi-h…	181817907	1
Caelo	Fosfato de codeína hemi-h…	18187902	3
Caelo	Fosfato de codeína hemi-h…	18187903	3
Caelo	Fosfato de codeína hemi-h…	18187906	3
Caelo	Fosfato de codeína hemi-h…	18187907	1
Caelo	Fosfato de codeína hemi-h…	18187908	1
Caelo	Fosfato de codeína hemi-h…	18187960	2
Caelo	Fosfato de codeína hemi-h…	20003804005	1
Caelo	Fosfato de codeína hemi-h…	20003804007	1
Caesar & Loretz GmbH	Fosfato de codeína hemi-h…	18187901	1
Caesar & Loretz GmbH	Fosfato de codeína hemi-h…	18187902	1
Caesar & Loretz GmbH	Fosfato de codeína hemi-h…	18187903	1
Caesar & Loretz GmbH	Fosfato de codeína hemi-h…	18187906	2
Caesar & Loretz Hilden	Fosfato de codeína hemi-h…	18187903	1
Euro OTC	Fosfato de codeína hemi-h…	CP04236	1
Euro/ Sanacorp	Fosfato de codeína hemi-h…	15F09-B02-315564	2
Fagron	Fosfato de codeína hemi-h…	11/19-N10	1
Fagron	Fosfato de codeína hemi-h…	12C05-N01	1
Fagron	Fosfato de codeína hemi-h…	13/27-N06	2
Fagron	Fosfato de codeína hemi-h…	13C11-N10	1
Fagron	Fosfato de codeína hemi-h…	13E21-N04	1
Fagron	Fosfato de codeína hemi-h…	15B17-B99-304623	2
Fagron	Fosfato de codeína hemi-h…	15F09-B02	1
Fagron	Fosfato de codeína hemi-h…	15F09-B02-310520	2
Fagron	Fosfato de codeína hemi-h…	15F09-B02-314033	1
Fagron	Fosfato de codeína hemi-h…	1615I-01279	1
Fagron	Fosfato de codeína hemi-h…	16E17-B05-324109	4
Fagron	Fosfato de codeína hemi-h…	17L22-B03-343752	1
Fagron	Fosfato de codeína hemi-h…	18D03-B01	1
Fagron	Fosfato de codeína hemi-h…	21D30-F01	1
Fagron	Fosfato de codeína hemi-h…	21D30-F01-380923	1
Fagron	Fosfato de codeína hemi-h…	5040218D	3
Fagron	Fosfato de codeína hemi-h…	913I-01279	1
Fagron	Fosfato de codeína hemi-h…	B01-3612302	2
Fagron	Fosfato de codeína hemi-h…	F04-3825805	1
Gehe	Fosfato de codeína hemi-h…	15350710	1
Merck	Fosfato de codeína hemi-h…	120765	1
Th. Geyer	Fosfato de codeína hemi-h…	67038	1
Th. Geyer	Fosfato de codeína hemi-h…	67054	31
Th. Geyer	Fosfato de codeína hemi-h…	70533	22

- 235 932 spectra from 1515 *Apo-Ident* customers from a total of 49 209 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fosfato de codeína hemi-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fosfato de codeína hemi-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	320	0	201 764
Type C	0	134	1	235 932

The substance/substance group *Fosfato de codeína hemi-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	99.2593 % (> 97.0370 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21148	21148	0,00	143,46
21150	21150	0,00	144,29
21152	21152	0,00	140,13
22407	22407	0,00	136,29
22425	22425	0,00	143,67
23466	23466	0,00	144,22
23469	23469	0,00	141,61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fosfato dibásico de clindamicina 2**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10003687-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fosfato dibásico de clindamicina 2; Clindamycini phosphas

Special notes

When selecting the *Fosfato dibásico de clindamicina 2* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fosfato dibásico de clindamicina 2	10	3	8

Second-stage model

For differentiation of the substance/substance group *Fosfato dibásico de clindamicina 2* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fosfato dibásico de clindamicina 2* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	66,87	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fosfato dibásico de clindamicina 2* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fosfato dibásico de clindamicina 2*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fosfato dibásico de clind…	13166605	21063	40	1403485
Caelo	Fosfato dibásico de clind…	13166605	21116	40	20130624
Caelo	Fosfato dibásico de clind…	14257305	21798	60	AR-15-FG-015412-01
Caelo	Fosfato dibásico de clind…	15435801	22312	60	AR-16-FG-009129-01
Caelo	Fosfato dibásico de clind…	163265	23055	40	20161214*
Caelo	Fosfato dibásico de clind…	16326504	23586	40	AR-17-FG-022557-01
Caelo	Fosfato dibásico de clind…	20002497001	25389	40	20200922
Caelo	Fosfato dibásico de clind…	21003094	25849	50	20211007*
Caelo	Fosfato dibásico de clind…	22000385	26022	40	20220317*
Caelo	Fosfato dibásico de clind…	22001647	26246	40	20220622*
Caelo	Fosfato dibásico de clind…	22001647	26246SI	20	20220622*
Caelo	Fosfato dibásico de clind…	24000953	27242	40	20240529*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 510 spectra of 12 reference samples from the substance/substance group *Fosfato dibásico de clindamicina 2*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 452 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Fosfato dibásico de clindamicina 2*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fosfato dibásico de clind…	172964	24047	40
Caelo	Fosfato dibásico de clind…	191224	24729	40
Caelo	Fosfato dibásico de clind…	23001027	26846	40
Caelo	Fosfato dibásico de clind…	22000385	26022SI†	10
Caelo	Fosfato dibásico de clind…	23001027	26846SI	20

- 201 934 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 18 spectra from 11 *Apo-Ident* customers from 9 batches from the substance/substance group *Fosfato dibásico de clindamicina 2*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fosfato dibásico de clind…	23001027002	1
Caelo	Fosfato dibásico de clind…	14257305	1
Caelo	Fosfato dibásico de clind…	16326507	1
Caelo	Fosfato dibásico de clind…	17344101	6
Caelo	Fosfato dibásico de clind…	17344102	1
Caelo	Fosfato dibásico de clind…	19122402	3
Caelo	Fosfato dibásico de clind…	22000385002	1
Caesar & Loretz GmbH	Fosfato dibásico de clind…	19122401	1
Caesar & Loretz GmbH	Fosfato dibásico de clind…	19122402	2
Noweda	Fosfato dibásico de clind…	23001027001	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 249 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fosfato dibásico de clindamicina 2* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fosfato dibásico de clindamicina 2* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	510	0	152 452
Type B	0	150	0	201 934
Type C	0	18	0	236 049

The substance/substance group *Fosfato dibásico de clindamicina 2* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21063	21063	0,00	117,13
21116	21063	2,97	117,06
21798	21798	0,00	118,60
22312	22312	0,00	120,42
23055	23055	0,00	133,13
23586	23586	0,00	142,35
25389	23586	64,84	129,41
25849	25849	0,00	134,65
26022	26022	0,00	149,95
26246	26246	0,00	145,83
27242	27242	0,00	100,63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fosfato dibásico de sódio di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005937-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fosfato dibásico de sódio di-hidratado; Natrii dihydrogenophosphas dihydricus

Special notes

When selecting the *Fosfato dibásico de sódio di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fosfato dibásico de sódio di-hidratado	4	3	10

Second-stage model

For differentiation of the substance/substance group *Fosfato dibásico de sódio di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fosfato dibásico de sódio di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	73,79	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fosfato dibásico de sódio di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fosfato dibásico de sódio di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fosfato dibásico de sódio…	22001753	26560	40	20220706*
Caelo	Fosfato dibásico de sódio…	22001753	26560SI	20	20220706*
Caelo	Fosfato dibásico de sódio…	24001049	27310	30	20240502*
Euro OTC	Fosfato dibásico de sódio…	2106004	25786	50	20210624*
Euro OTC	Fosfato dibásico de sódio…	2204005	26101	40	20220517*
Euro OTC	Fosfato dibásico de sódio…	2204005	26101SI	20	20220517*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 6 reference samples from the substance/substance group *Fosfato dibásico de*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

sódio di-hidratado. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 762 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Fosfato dibásico de sódio di-hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fosfato dibásico de sódio…	21001537	25802	50
Euro OTC	Fosfato dibásico de sódio…	2109011	25817	50
Euro OTC	Fosfato dibásico de sódio…	2307018	26860	40
Euro OTC	Fosfato dibásico de sódio…	2307018	26860SI	20

- 201 924 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 16 *Apo-Ident* customers from 10 batches from the substance/substance group *Fosfato dibásico de sódio di-hidratado*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fosfato dibásico de sódio…	22001753006	2
	Fosfato dibásico de sódio…	22001753011	2
	Fosfato dibásico de sódio…	2204005-01	1
Caelo	Fosfato dibásico de sódio…	12198506	1
Caelo	Fosfato dibásico de sódio…	12198510	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fosfato dibásico de sódio…	12198517	2
Caelo	Fosfato dibásico de sódio…	13D08-N25	1
Euro OTC	Fosfato dibásico de sódio…	1209004-01	2
Euro OTC	Fosfato dibásico de sódio…	1305028-01	2
Fagron	Fosfato dibásico de sódio…	12L05-N05	1
Gehe	Fosfato dibásico de sódio…	12198510	1

- 236 051 spectra from 1515 *Apo-Ident* customers from a total of 49 248 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fosfato dibásico de sódio di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fosfato dibásico de sódio di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	160	0	201 924
Type C	0	16	0	236 051

The substance/substance group *Fosfato dibásico de sódio di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25786	25786	0,00	97,92
26101	26101	0,00	58,31
26560	26560	0,00	55,78
27310	27310	0,00	53,33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fosfato dissódico de prednisolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20212-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fosfato dissódico de prednisolona; Prednisoloni natrii phosphas

Special notes

When selecting the *Fosfato dissódico de prednisolona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fosfato dissódico de prednisolona	9	3	117

Second-stage model

For differentiation of the substance/substance group *Fosfato dissódico de prednisolona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fosfato dissódico de prednisolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	66,63	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fosfato dissódico de prednisolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fosfato dissódico de prednisolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fosfato dissódico de pred…	13304703	20923	40	20130904
Caelo	Fosfato dissódico de pred…	13304704	21412	60	1411052
Caelo	Fosfato dissódico de pred…	16174715	23271	40	20160930
Caelo	Fosfato dissódico de pred…	20002455003	25393	40	20200824
Caelo	Fosfato dissódico de pred…	20002455003	25393SI	40	20200824
Fagron	Fosfato dissódico de pred…	14E07-B06-295251	21571	60	20140623
Fagron	Fosfato dissódico de pred…	18D23-B08-351348	24293	40	1812421
Fagron	Fosfato dissódico de pred…	18K27-B04-363613	25375	40	20190828
Fagron	Fosfato dissódico de pred…	21E25-F03-378586	25912	40	2204384
Fagron	Fosfato dissódico de pred…	21E25-F03-378586	25912SI	30	2204384
Fagron	Fosfato dissódico de pred…	24A29-B02-233778	27175	40	20240219
Fagron	Fosfato dissódico de pred…	24A29-B02-233778	27175SI	40	20240219

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 510 spectra of 12 reference samples from the substance/substance group *Fosfato dissódico de prednisolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 452 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 5 reference samples from the substance/substance group *Fosfato dissódico de prednisolona*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fosfato dissódico de pred…	181940	24905	40
Caelo	Fosfato dissódico de pred…	21003179007	25987	40
Fagron	Fosfato dissódico de pred…	16I14-B03-328918	23270	40
Caelo	Fosfato dissódico de pred…	21003179007	25987SI	40
Fagron	Fosfato dissódico de pred…	18K27-B04-363613	25375SI†	40

- 201 884 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 294 spectra from 119 *Apo-Ident* customers from 125 batches from the substance/substance group *Fosfato dissódico de prednisolona*.

- Among them are spectra of independent samples from 117 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Fosfato dissódico de pred…	21E25-F03-378592	5
	Fosfato dissódico de pred…	21K16-B16-226142	3
	Fosfato dissódico de pred…	23001195003	1
	Fosfato dissódico de pred…	23001195004	1
	Fosfato dissódico de pred…	23003063002	1
	Fosfato dissódico de pred…	23003063003	1
	Fosfato dissódico de pred…	24A29-B02-233778	1
Alte Apotheke	Fosfato dissódico de pred…	15K27B09-318738	1
Caelo	Fosfato dissódico de pred…	14196602	1
Caelo	Fosfato dissódico de pred…	15199602	2
Caelo	Fosfato dissódico de pred…	15199603	1
Caelo	Fosfato dissódico de pred…	16174701	1
Caelo	Fosfato dissódico de pred…	16174702	1
Caelo	Fosfato dissódico de pred…	16174706	1
Caelo	Fosfato dissódico de pred…	16174710	1
Caelo	Fosfato dissódico de pred…	17077502	2
Caelo	Fosfato dissódico de pred…	17077503	1
Caelo	Fosfato dissódico de pred…	17077508	2
Caelo	Fosfato dissódico de pred…	18024602	1
Caelo	Fosfato dissódico de pred…	18024604	2
Caelo	Fosfato dissódico de pred…	18194001	2
Caelo	Fosfato dissódico de pred…	18194002	6
Caelo	Fosfato dissódico de pred…	18194003	3
Caelo	Fosfato dissódico de pred…	18194006	9
Caelo	Fosfato dissódico de pred…	18194007	2
Caelo	Fosfato dissódico de pred…	18194010	1
Caelo	Fosfato dissódico de pred…	18194011	2
Caelo	Fosfato dissódico de pred…	19129302	2
Caelo	Fosfato dissódico de pred…	19129304	8
Caelo	Fosfato dissódico de pred…	19129306	4
Caelo	Fosfato dissódico de pred…	192754002	2
Caelo	Fosfato dissódico de pred…	19275402	2
Caelo	Fosfato dissódico de pred…	19275403	3
Caelo	Fosfato dissódico de pred…	20001707001	2
Caelo	Fosfato dissódico de pred…	20001707002	2
Caelo	Fosfato dissódico de pred…	20001707003	2
Caelo	Fosfato dissódico de pred…	20001707008	2
Caelo	Fosfato dissódico de pred…	20002455002	3
Caelo	Fosfato dissódico de pred…	20002455003	1
Caelo	Fosfato dissódico de pred…	20003761001	1
Caelo	Fosfato dissódico de pred…	20003761002	4
Caelo	Fosfato dissódico de pred…	20003761003	1
Caelo	Fosfato dissódico de pred…	2001707001	1
Caelo	Fosfato dissódico de pred…	21000431001	1
Caelo	Fosfato dissódico de pred…	21000431002	2
Caelo	Fosfato dissódico de pred…	21000431003	1
Caelo	Fosfato dissódico de pred…	21000431006	1
Caelo	Fosfato dissódico de pred…	21001330002	2
Caelo	Fosfato dissódico de pred…	21001330003	1
Caelo	Fosfato dissódico de pred…	2100317009	1
Caelo	Fosfato dissódico de pred…	21003179002	2
Caelo	Fosfato dissódico de pred…	21003179003	2
Caelo	Fosfato dissódico de pred…	21003179004	4
Caelo	Fosfato dissódico de pred…	21003179007	1
Caelo	Fosfato dissódico de pred…	21003179008	4
Caelo	Fosfato dissódico de pred…	21003179009	3
Caelo	Fosfato dissódico de pred…	22000048001	2
Caelo	Fosfato dissódico de pred…	22000048005	1
Caelo	Fosfato dissódico de pred…	2200048002	1
Caelo	Fosfato dissódico de pred…	2200048003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fosfato dissódico de pred…	23001195001	1
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	19129302	1
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	19275402	1
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	19129306	1
Caesar & Loretz GmbH/Gehe	Fosfato dissódico de pred…	22000048003	1
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	21000431001	2
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	21003179004	1
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	21000431001	2
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	21003179004	1
Caesar & Loretz GmbH…	Fosfato dissódico de pred…	22000048003	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	18194006	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	19129302	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	19129304	4
Caesar & Loretz GmbH	Fosfato dissódico de pred…	19275402	2
Caesar & Loretz GmbH	Fosfato dissódico de pred…	19275403	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	20001707002	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	20002455002	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	20003761002	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	21000431001	2
Caesar & Loretz GmbH	Fosfato dissódico de pred…	21000431002	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	21000431006	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	21003179003	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	21003179007	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	21003179008	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	22000048002	1
Caesar & Loretz GmbH	Fosfato dissódico de pred…	22000048003	2
Caesar & Loretz/Gehe…	Fosfato dissódico de pred…	20001707001	1
Caesar & Loretz/Gehe	Fosfato dissódico de pred…	18194001	1
Fagron	Fosfato dissódico de pred…	11C18-N11	1
Fagron	Fosfato dissódico de pred…	11K11-N11	2
Fagron	Fosfato dissódico de pred…	12H30-N08	3
Fagron	Fosfato dissódico de pred…	13/27-N01	1
Fagron	Fosfato dissódico de pred…	13A10-N04	3
Fagron	Fosfato dissódico de pred…	13C26N06	1
Fagron	Fosfato dissódico de pred…	13H19N04	1
Fagron	Fosfato dissódico de pred…	13I27-N01	4
Fagron	Fosfato dissódico de pred…	14E07-B06-295251	4
Fagron	Fosfato dissódico de pred…	14E07-B06-295253	1
Fagron	Fosfato dissódico de pred…	14G30-B09	1
Fagron	Fosfato dissódico de pred…	14G30-B09-303012	7
Fagron	Fosfato dissódico de pred…	14g30-b09-303014	1
Fagron	Fosfato dissódico de pred…	14G30-B09-303014	4
Fagron	Fosfato dissódico de pred…	15f29-b11-309694	1
Fagron	Fosfato dissódico de pred…	15F29-B11-309694	1
Fagron	Fosfato dissódico de pred…	15J01-B02	4
Fagron	Fosfato dissódico de pred…	15J01-B02-312722	5
Fagron	Fosfato dissódico de pred…	15J01-B02-313610	3
Fagron	Fosfato dissódico de pred…	15J01-B02-317180	2
Fagron	Fosfato dissódico de pred…	15K27-B09	4
Fagron	Fosfato dissódico de pred…	15k27-b09-318738	1
Fagron	Fosfato dissódico de pred…	15K27-B09-318738	3
Fagron	Fosfato dissódico de pred…	15K27-B09-322162	1
Fagron	Fosfato dissódico de pred…	15K27-B09-322163	3
Fagron	Fosfato dissódico de pred…	15K27B09-326263	1
Fagron	Fosfato dissódico de pred…	15K27-B09-326263	3
Fagron	Fosfato dissódico de pred…	16/14-B03-328169	1
Fagron	Fosfato dissódico de pred…	16I14-B03	2
Fagron	Fosfato dissódico de pred…	16I14-B03-328169	2
Fagron	Fosfato dissódico de pred…	16I14-B03-328918	3
Fagron	Fosfato dissódico de pred…	17/27-b03-342560	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Fosfato dissódico de pred…	17/27-B03-345405	1
Fagron	Fosfato dissódico de pred…	17B08-B05	1
Fagron	Fosfato dissódico de pred…	17B08B05337466	1
Fagron	Fosfato dissódico de pred…	17B08-B05-337466	4
Fagron	Fosfato dissódico de pred…	17B08-B05-340336	2
Fagron	Fosfato dissódico de pred…	17I12-B03-354549	1
Fagron	Fosfato dissódico de pred…	17I27-B03	2
Fagron	Fosfato dissódico de pred…	17I27-B03-342560	1
Fagron	Fosfato dissódico de pred…	17I27-B03-344246	3
Fagron	Fosfato dissódico de pred…	17I27-B03-345405	1
Fagron	Fosfato dissódico de pred…	17I27-B03-348462	1
Fagron	Fosfato dissódico de pred…	17I27-B03-354549	2
Fagron	Fosfato dissódico de pred…	18B02-B04-352053	1
Fagron	Fosfato dissódico de pred…	18D23-B08-350207	1
Fagron	Fosfato dissódico de pred…	18D23-B08-351348	1
Fagron	Fosfato dissódico de pred…	18D23-B08-352211	1
Fagron	Fosfato dissódico de pred…	18K27-B04	2
Fagron	Fosfato dissódico de pred…	18K27-B04-363611	2
Fagron	Fosfato dissódico de pred…	18K27-B04-363613	1
Fagron	Fosfato dissódico de pred…	19118D23-B08-350207	1
Fagron	Fosfato dissódico de pred…	21E25-F03-378585	2
Fagron	Fosfato dissódico de pred…	21E25-F03-378591	1
Fagron	Fosfato dissódico de pred…	21K16-B16-226142	1
Fagron	Fosfato dissódico de pred…	NU1356	1
Fagron	Fosfato dissódico de pred…	PSP002/0816	2
Fagron	Fosfato dissódico de pred…	PSP004/0117	1
Gehe	Fosfato dissódico de pred…	22002348005	1
Newchem spa	Fosfato dissódico de pred…	15J01-B02-313610	2
Noweda	Fosfato dissódico de pred…	22002348005	1
Noweda	Fosfato dissódico de pred…	23001195002	1
Noweda	Fosfato dissódico de pred…	23001195003	2
Phoenix	Fosfato dissódico de pred…	192754004	1
Sanacorp	Fosfato dissódico de pred…	19129304	1
Sanacorp	Fosfato dissódico de pred…	21000431002	1
Sidonia	Fosfato dissódico de pred…	17I27-B03-342560	1
Sidonia	Fosfato dissódico de pred…	17I27-B03-344246	1
Sidonia	Fosfato dissódico de pred…	17I27-B03-345405	6
Symbiotica / Noweda	Fosfato dissódico de pred…	18K27-B04-3636101	1
Symbiotica / Noweda	Fosfato dissódico de pred…	B04-3636101	1

- 235 773 spectra from 1515 *Apo-Ident* customers from a total of 49 134 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fosfato dissódico de prednisolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fosfato dissódico de prednisolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	510	0	152 452
Type B	0	200	0	201 884
Type C	0	291	3	235 773

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Fosfato dissódico de prednisolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.9796 % (> 97.9592 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20923	21412	17,14	153,54
21412	21412	0,00	147,00
21571	21412	21,11	143,37
23271	21412	14,96	160,79
24293	24293	0,00	130,92
25375	24293	78,53	152,65
25393	21412	13,94	148,06
25912	25912	0,00	163,42
27175	21412	50,77	164,53

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fosfato sódico de riboflavina hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20948-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fosfato sódico de riboflavina hidratado; Riboflavini natrii phosphas hydricum

Special notes

When selecting the *Fosfato sódico de riboflavina hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fosfato sódico de riboflavina hidratado	8	3	3

Second-stage model

For differentiation of the substance/substance group *Fosfato sódico de riboflavina hidratado* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fosfato sódico de riboflavina hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	40,36	–
Carbômero	41,52	41,89
Citrato de magnésio	47,70	34,91
⋮	⋮	⋮
Fosfato de Mg-Ca-K-colamina	>50	109,18
Sulfato de gentamicina	>50	112,26
Sulfato de neomicina	>50	223,58
Sulfato de tobramicina	>50	283,06
Gluconato de zinco	>50	344,56
Tetraborato de sódio	>50	650,64
Finasterida	>50	747,82

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fosfato sódico de riboflavina hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fosfato sódico de riboflavina hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Fosfato sódico de ribofla…	2306014	26856	40	20230831*
Fagron	Fosfato sódico de ribofla…	13I26-N06	20948	40	1403705
Fagron	Fosfato sódico de ribofla…	15J02-B03-313137	22269	60	AR-16-FG-009883-02
Fagron	Fosfato sódico de ribofla…	17A03-B01-335897	23713	40	AR-18-FG-000920-01
Fagron	Fosfato sódico de ribofla…	20L02-B02-202655	25494	40	2105284
Fagron	Fosfato sódico de ribofla…	21E19-B01-213684	26162	40	20210702
Fagron	Fosfato sódico de ribofla…	22D20-B02-221099	26461	40	20220625
Fagron	Fosfato sódico de ribofla…	23E16-B05-229478	26829	40	20230602
Fagron	Fosfato sódico de ribofla…	23E16-B05-229478	26829SI	20	20230602

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Fosfato sódico de riboflavina hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 165 spectra of 5 reference samples from the substance/substance group *Fosfato sódico de riboflavina hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Fosfato sódico de ribofla…	2302008	26659	40
Fagron	Fosfato sódico de ribofla…	14J31-B07-300519	21707	45
Fagron	Fosfato sódico de ribofla…	17H03-B13-347175	24113	40
Euro OTC	Fosfato sódico de ribofla…	2302008	26659SI	20
Fagron	Fosfato sódico de ribofla…	21E19-B01-213684	26162SI†	20

- 201 919 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 6 spectra from 1 *Apo-Ident* customers from 5 batches from the substance/substance group *Fosfato sódico de riboflavina hidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Fosfato sódico de ribofla…	20H27	1
Fagron	Fosfato sódico de ribofla…	20H27-B07-201994	1
Fagron	Fosfato sódico de ribofla…	20L02-B02-202655	1
Fagron	Fosfato sódico de ribofla…	21E19-B01-213684	2
Sigma Aldrich	Fosfato sódico de ribofla…	MKCG3538	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fosfato sódico de riboflavina hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fosfato sódico de riboflavina hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	165	0	201 919
Type C	0	6	0	236 061

The substance/substance group *Fosfato sódico de riboflavina hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.3636 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20948	20948	0,00	52,83
22269	22269	0,00	66,92
23713	23713	0,00	93,03
25494	25494	0,00	98,78
26162	25494	17,70	113,23
26461	25494	9,76	102,30
26829	25494	47,32	129,02
26856	26856	0,00	82,38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Frutose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20074-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Frutose; Fructosum

Special notes

When selecting the *Frutose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Frutose	7	21	289

Second-stage model

For differentiation of the substance/substance group *Frutose* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Frutose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	62,28	41,66
⋮	⋮	⋮
Glicerofosfato de cálcio	>50	35,61
Riboflavina	>50	40,22
Sulfato de colistina	>50	41,45
Anfotericina B	>50	49,72
Tosilcloramida sódica	>50	56,26
Bacitracina	>50	57,74
SyrSpend® SF pH4 neo	>50	61,09
Amido de trigo	>50	64,33
Amido de arroz	>50	64,96
Pantotenato de cálcio	>50	65,30
SyrSpend® SF Alka	>50	68,05
Fécula de batata	>50	74,95
Nistatina	>50	77,90
Levedura de selênio	>50	78,65
SyrSpend® SF pH4	>50	79,21
Gelatina, branca	>50	84,34
Carmelose sódica	>50	85,76
Maltodextrina	>50	88,82
Goma arábica, dispersão seca	>50	91,47
Amido de milho	>50	99,85
Triancinolona	>50	99,92
Bromidrato de hioscina	>50	103,24
Cianocobalamina	>50	108,64
Ácido oxálico	>50	110,73
Estradiol hemi-hidratado	>50	112,00
Metilcobalamina	>50	161,71
Vitamina E acetato pó 50%	>50	168,94
Estriol	>50	169,06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Frutose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Frutose*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Frutose	160667	22481	60	20160425*
Caelo	Frutose	15084311	22490	40	20150316
Euro OTC	Frutose	1212015-01	21281	40	20130111
Euro OTC	Frutose	1509037	21934	60	20151027*
Euro OTC	Frutose	1512009	22292	60	20160113*
Euro OTC	Frutose	1701049	22986	40	20170213*
Fagron	Frutose	16H05-B01-326259	23018	40	20160926
Fagron	Frutose	16H05-B01-326259	23082	40	20160926

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 380 spectra of 8 reference samples from the substance/substance group *Frutose*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 582 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 921 spectra of 25 reference samples from the substance/substance group *Frutose*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Frutose	15271213	22583	40
Caelo	Frutose	171439	23422	40
Caelo	Frutose	182916	24364	40
Caelo	Frutose	191699	24739	40
Caelo	Frutose	21000686007	25931	40
Caelo	Frutose	23002084	27334	40
Euro OTC	Frutose	1604024	22547	41

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Frutose	1607030	22693	40
Euro OTC	Frutose	1705002	23391	40
Euro OTC	Frutose	1710034	23901	40
Euro OTC	Frutose	1803040	24087	40
Euro OTC	Frutose	1811018	24486	40
Euro OTC	Frutose	1906017	24792	40
Euro OTC	Frutose	1910020	24978	40
Euro OTC	Frutose	2006019	25298	40
Euro OTC	Frutose	2102008	25602	40
Euro OTC	Frutose	2203030	26037	40
Euro OTC	Frutose	2212011	26516	40
Euro OTC	Frutose	2309017	26996	40
Euro OTC	Frutose	2405018	27281	40
Fagron	Frutose	19C19-B02-361846	25057	40
Caelo	Frutose	171439	23673	40
Caelo	Frutose	21000686007	25931SI	10
Euro OTC	Frutose	2203030	26037SI	10
Euro OTC	Frutose	2212011	26516SI	20

- 201 163 spectra from a total of 4024 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1268 spectra from 321 *Apo-Ident* customers from 293 batches from the substance/substance group *Frutose*.

- Among them are spectra of independent samples from 289 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Frutose	2006019-02	2
	Frutose	2100068018	1
	Frutose	21000686027	1
	Frutose	22003150003	10
	Frutose	22003150007	1
	Frutose	22003150009	1
	Frutose	22003150016	2
	Frutose	22003150021	3
	Frutose	2200315003	1
	Frutose	2203030-01	2
	Frutose	2203030-02	1
	Frutose	2212011-01	6
	Frutose	2212011-02	4
	Frutose	23003368001	2
	Frutose	23003368002	1
	Frutose	2309017-01	2
	Frutose	FS2P00251808-S02	1
AHD	Frutose	FS2P00252305-190	1
Alliance Health 13.0...	Frutose	13C25-N03	1
Alliance health	Frutose	14E01-B04-293505	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Alliance health	Frutose	14K17-B99-300913	3
Alliance	Frutose	22003150002	2
Alliance	Frutose	2212011-01	1
Anzag	Frutose	18291602	1
apo-ident	Frutose	1607030-01	2
Beiersdorf	Frutose	14096208	1
Bombastus	Frutose	1710034-01	1
Caelo	Frutose	10051401	1
Caelo	Frutose	10071201	1
Caelo	Frutose	10087516	1
Caelo	Frutose	10381011	1
Caelo	Frutose	104H20	1
Caelo	Frutose	1081501	1
Caelo	Frutose	11071201	1
Caelo	Frutose	1114A03394	1
Caelo	Frutose	11258611	1
Caelo	Frutose	11258614	1
Caelo	Frutose	11258627	3
Caelo	Frutose	11258628	2
Caelo	Frutose	11I07-N06	1
Caelo	Frutose	12132301	2
Caelo	Frutose	12132305	5
Caelo	Frutose	12132309	2
Caelo	Frutose	12132310	1
Caelo	Frutose	12132313	5
Caelo	Frutose	12132314	5
Caelo	Frutose	12132317	2
Caelo	Frutose	12132320	1
Caelo	Frutose	12132322	2
Caelo	Frutose	12132325	3
Caelo	Frutose	121e29-n08	1
Caelo	Frutose	123456	1
Caelo	Frutose	1234567	1
Caelo	Frutose	12H01-N03	1
Caelo	Frutose	13041802	1
Caelo	Frutose	1309213394	1
Caelo	Frutose	13098902	3
Caelo	Frutose	13098904	1
Caelo	Frutose	13098906	4
Caelo	Frutose	13098909	1
Caelo	Frutose	13098911	1
Caelo	Frutose	13098913	4
Caelo	Frutose	13098914	2
Caelo	Frutose	13098915	1
Caelo	Frutose	13098917	3
Caelo	Frutose	13098918	1
Caelo	Frutose	13098922	1
Caelo	Frutose	130998922	1
Caelo	Frutose	13111705	1
Caelo	Frutose	13A28-N01	1
Caelo	Frutose	13E27-N07	1
Caelo	Frutose	14096201	2
Caelo	Frutose	14096202	1
Caelo	Frutose	14096203	1
Caelo	Frutose	14096205	3
Caelo	Frutose	14096207	1
Caelo	Frutose	14096208	2
Caelo	Frutose	14096210	1
Caelo	Frutose	14096211	1
Caelo	Frutose	14096219	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Frutose	14096223	5
Caelo	Frutose	14096224	2
Caelo	Frutose	14305201	1
Caelo	Frutose	14305203	2
Caelo	Frutose	14305204	1
Caelo	Frutose	14305206	1
Caelo	Frutose	14E01-B04-297098	1
Caelo	Frutose	1503045-01	2
Caelo	Frutose	15049703	1
Caelo	Frutose	15084301	3
Caelo	Frutose	15084305	3
Caelo	Frutose	15084308	2
Caelo	Frutose	15084311	2
Caelo	Frutose	15084312	2
Caelo	Frutose	1509037-01	2
Caelo	Frutose	152711201	1
Caelo	Frutose	15271201	3
Caelo	Frutose	15271205	7
Caelo	Frutose	15271208	2
Caelo	Frutose	15271209	4
Caelo	Frutose	15271213	6
Caelo	Frutose	15271214	2
Caelo	Frutose	15271215	3
Caelo	Frutose	15A16-B07	1
Caelo	Frutose	15A16-B07-305241	1
Caelo	Frutose	1604024-01	1
Caelo	Frutose	16066101	2
Caelo	Frutose	16066103	6
Caelo	Frutose	16066106	20
Caelo	Frutose	16066107	9
Caelo	Frutose	1607030-01	1
Caelo	Frutose	1610033-01	2
Caelo	Frutose	16283910	7
Caelo	Frutose	17007701	5
Caelo	Frutose	17007702	1
Caelo	Frutose	17007706	1
Caelo	Frutose	17007707	2
Caelo	Frutose	17007708	1
Caelo	Frutose	1701034-01	1
Caelo	Frutose	170104901	1
Caelo	Frutose	1705002-01	1
Caelo	Frutose	1710034-01	3
Caelo	Frutose	17143902	12
Caelo	Frutose	1714390210087516	1
Caelo	Frutose	17143903	2
Caelo	Frutose	17143904	10
Caelo	Frutose	17346404	29
Caelo	Frutose	17346405	1
Caelo	Frutose	17346405P-180831-1	1
Caelo	Frutose	17346405P-190325-2	1
Caelo	Frutose	17346405P-190718-1	1
Caelo	Frutose	17346406	1
Caelo	Frutose	17346411	2
Caelo	Frutose	18021501	1
Caelo	Frutose	1803040-01	4
Caelo	Frutose	18061801	1
Caelo	Frutose	18062005	1
Caelo	Frutose	18082002	9
Caelo	Frutose	18082005	38
Caelo	Frutose	18082006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Frutose	18082011	4
Caelo	Frutose	18082012	4
Caelo	Frutose	1811018-01	1
Caelo	Frutose	1829102	1
Caelo	Frutose	18291602	40
Caelo	Frutose	18291603	1
Caelo	Frutose	18291603P-191223-2	1
Caelo	Frutose	18291605	2
Caelo	Frutose	18291609	7
Caelo	Frutose	18291611P-200319-9	1
Caelo	Frutose	18291612	2
Caelo	Frutose	18291613	5
Caelo	Frutose	18291614	1
Caelo	Frutose	18291620	2
Caelo	Frutose	1906017-01	7
Caelo	Frutose	1910020-01	2
Caelo	Frutose	191699005	1
Caelo	Frutose	19169903	13
Caelo	Frutose	19169904	8
Caelo	Frutose	19169905	1
Caelo	Frutose	192965002	7
Caelo	Frutose	192965008	16
Caelo	Frutose	192965009	1
Caelo	Frutose	20003599001	2
Caelo	Frutose	20003599011	5
Caelo	Frutose	20003599012	6
Caelo	Frutose	20081402	1
Caelo	Frutose	2100066022	1
Caelo	Frutose	21000686003	1
Caelo	Frutose	21000686007	5
Caelo	Frutose	21000686009	2
Caelo	Frutose	21000686015	5
Caelo	Frutose	21000686016	1
Caelo	Frutose	21000686018	2
Caelo	Frutose	21000686020	3
Caelo	Frutose	21000686022	11
Caelo	Frutose	21000686024	8
Caelo	Frutose	2102008-02	3
Caelo	Frutose	21051303	1
Caelo	Frutose	2117E-03394	1
Caelo	Frutose	22003150002	4
Caelo	Frutose	22003150003	3
Caelo	Frutose	22003150007	4
Caelo	Frutose	220425C	1
Caelo	Frutose	23021708	1
Caelo	Frutose	31031401	1
Caelo	Frutose	31101810	1
Caelo	Frutose	3313U-03394	1
Caelo	Frutose	5061503	1
Caelo	Frutose	5081701	1
Caelo	Frutose	7051304	1
Caelo	Frutose	7111401	1
Caelo	Frutose	716090F	1
Caelo	Frutose	9031504	1
Caelo	Frutose	9061804	1
Caelo	Frutose	92965008	1
Caesar & Loretz / Gehe	Frutose	18082012	1
Caesar & Loretz GmbH...	Frutose	19169904	1
Caesar & Loretz GmbH...	Frutose	18291605	2
Caesar & Loretz GmbH...	Frutose	18291613	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Frutose	20003599012	1
Caesar & Loretz GmbH...	Frutose	18291602	1
Caesar & Loretz GmbH...	Frutose	18291609	1
Caesar & Loretz GmbH/AHD	Frutose	18291602	1
Caesar & Loretz GmbH...	Frutose	21000686027	1
Caesar & Loretz GmbH/Gehe	Frutose	20003599011	1
Caesar & Loretz GmbH/Gehe	Frutose	21000686022	1
Caesar & Loretz GmbH...	Frutose	18082012	1
Caesar & Loretz GmbH...	Frutose	20003599001	1
Caesar & Loretz GmbH...	Frutose	18291602	1
Caesar & Loretz GmbH...	Frutose	19169904	4
Caesar & Loretz GmbH	Frutose	16283910	1
Caesar & Loretz GmbH	Frutose	18082005	4
Caesar & Loretz GmbH	Frutose	18082011	1
Caesar & Loretz GmbH	Frutose	18291602	24
Caesar & Loretz GmbH	Frutose	18291609	2
Caesar & Loretz GmbH	Frutose	18291613	1
Caesar & Loretz GmbH	Frutose	18307407	1
Caesar & Loretz GmbH	Frutose	191699008	1
Caesar & Loretz GmbH	Frutose	19169903	6
Caesar & Loretz GmbH	Frutose	19169904	1
Caesar & Loretz GmbH	Frutose	19169905	1
Caesar & Loretz GmbH	Frutose	192965002	4
Caesar & Loretz GmbH	Frutose	192965008	4
Caesar & Loretz GmbH	Frutose	20003599001	1
Caesar & Loretz GmbH	Frutose	20003599011	4
Caesar & Loretz GmbH	Frutose	20003599012	1
Caesar & Loretz GmbH	Frutose	21000686007	6
Caesar & Loretz GmbH	Frutose	21000686009	2
Caesar & Loretz GmbH	Frutose	21000686015	1
Caesar & Loretz GmbH	Frutose	21000686016	1
Caesar & Loretz GmbH	Frutose	21000686020	1
Caesar & Loretz GmbH	Frutose	21000686022	3
Caesar & Loretz GmbH	Frutose	21000686024	1
Caesar & Loretz GmbH	Frutose	22003150003	1
Caesar & Loretz GmbH	Frutose	22003150007	1
Caesar & Loretz/Geil...	Frutose	18291602	1
Caesar u. Loretz GmbH	Frutose	18082002	1
Caesar u. Loretz GmbH	Frutose	19169904	1
Caesar&Loretz/Noweda	Frutose	18082005	1
Ebert & Jacobi 08.08.16	Frutose	1604024-01	1
Eigen	Frutose	122F21	1
Eigen	Frutose	127D21	1
Eigen	Frutose	128I20	1
Eigenherstellung Defektur	Frutose	5082101	1
Eigenherstellung	Frutose	112K21	1
EuRho / Fiebig	Frutose	1910020-01	1
EuRho/Alliance	Frutose	2006019-01	2
Eurho/Gehe	Frutose	190601701	1
EuRho/Noweda	Frutose	1604024-01	1
EuRho	Frutose	1503045-01	1
EuRho	Frutose	1509037-01	4
EuRho	Frutose	1705002-01	2
EuRho	Frutose	171003401	2
EuRho	Frutose	1803040-01	1
EuRho	Frutose	2006019-19	1
Euro OTC	Frutose	1201017-01	2
Euro OTC	Frutose	1205022-01	1
Euro OTC	Frutose	1209010-01	1
Euro OTC	Frutose	121201-01pzn	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Frutose	1212015-01	2
Euro OTC	Frutose	12E29-N08	1
Euro OTC	Frutose	1307022-01	4
Euro OTC	Frutose	140100401	1
Euro OTC	Frutose	1401004-01	4
Euro OTC	Frutose	141000901	2
Euro OTC	Frutose	1410009-01	6
Euro OTC	Frutose	148890	1
Euro OTC	Frutose	1503045-01	7
Euro OTC	Frutose	1509037-01	7
Euro OTC	Frutose	1512009-01	9
Euro OTC	Frutose	1604024-01	4
Euro OTC	Frutose	1607030-01	17
Euro OTC	Frutose	1610033	1
Euro OTC	Frutose	1610033-01	12
Euro OTC	Frutose	1701049-01	14
Euro OTC	Frutose	170500201	1
Euro OTC	Frutose	1705002-01	10
Euro OTC	Frutose	171003401	1
Euro OTC	Frutose	1710034-01	33
Euro OTC	Frutose	180304001	1
Euro OTC	Frutose	1803040-01	34
Euro OTC	Frutose	1803040-012	1
Euro OTC	Frutose	1803040-02	3
Euro OTC	Frutose	1803040-03	1
Euro OTC	Frutose	1803040-1	1
Euro OTC	Frutose	18082002	1
Euro OTC	Frutose	181018-01	1
Euro OTC	Frutose	1811018	1
Euro OTC	Frutose	1811018-01	38
Euro OTC	Frutose	19006017-01	1
Euro OTC	Frutose	1906017-01	28
Euro OTC	Frutose	1910020-01	22
Euro OTC	Frutose	2006019-01	18
Euro OTC	Frutose	2102008-002	1
Euro OTC	Frutose	2102008-01	15
Euro OTC	Frutose	2102008-02	6
Euro OTC	Frutose	2203030_01	1
Euro OTC	Frutose	220303001	3
Euro OTC	Frutose	2203030-01	17
Euro OTC	Frutose	2212011-02	2
Euro OTC	Frutose	252207-4204	1
Euro OTC	Frutose	2731	1
Euro OTC	Frutose	AD15190330	1
Euro OTC	Frutose	AD16C91215	1
Euro OTC	Frutose	FS2P00251707-304	1
Euro OTC	Frutose	FS2P00251802-122	1
euro//Noweda	Frutose	1509037-01	1
euro//Noweda	Frutose	1710034-01	1
Euro/Gehe	Frutose	1604024-01	1
Euro/Gehe	Frutose	1607030-01	1
Euro/Krieger	Frutose	1906017-01	2
Euro/Noweda	Frutose	1610033-01	2
euroct/gehe	Frutose	1212015-01	1
Europh/Ph	Frutose	1906017-01	1
Europh/Ph	Frutose	1910020-01	2
Fagron	Frutose	1107-N06	1
Fagron	Frutose	1170	1
Fagron	Frutose	12A26-N04	1
Fagron	Frutose	12E29-N08	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Frutose	12H01-N03	1
Fagron	Frutose	12Ho1-N03	1
Fagron	Frutose	12K28-N06	2
Fagron	Frutose	13098906	1
Fagron	Frutose	1312A-03394	1
Fagron	Frutose	13A28-N01	10
Fagron	Frutose	13C25-N03	3
Fagron	Frutose	13E27-n07	1
Fagron	Frutose	13E27-N07	2
Fagron	Frutose	13J18-B06	2
Fagron	Frutose	13J18-B06-286894	1
Fagron	Frutose	13J18B06286896	1
Fagron	Frutose	13J18-B06-286899	1
Fagron	Frutose	13J18-B06-292061	1
Fagron	Frutose	14E01-B04	3
Fagron	Frutose	14E01-B04-29350	1
Fagron	Frutose	14E01-B04-293505	6
Fagron	Frutose	14E01B04293506	1
Fagron	Frutose	14E01-B04-297098	2
Fagron	Frutose	14E1-B04-293506	1
Fagron	Frutose	14k17-B99	2
Fagron	Frutose	14K17-B99	2
Fagron	Frutose	14K17-B99-300913	1
Fagron	Frutose	15/21-B01	1
Fagron	Frutose	15/21-B01-312700	1
Fagron	Frutose	15/21-B01-323021	1
Fagron	Frutose	1521-B01-323021	1
Fagron	Frutose	15A16-B07	1
Fagron	Frutose	15A16-B07-303124	2
Fagron	Frutose	15A16-B07-305241	1
Fagron	Frutose	15A16-B07-308950	3
Fagron	Frutose	15I21-B01	1
Fagron	Frutose	15I21-B01-323020	1
Fagron	Frutose	15I21-B01-323021	5
Fagron	Frutose	15l21-B01-312701	2
Fagron	Frutose	15l21-B01-323021	1
Fagron	Frutose	16H05-B01	2
Fagron	Frutose	16H05-B01-326259	1
Fagron	Frutose	16H05-B01-330164	3
Fagron	Frutose	17007701	1
Fagron	Frutose	1705002-01	1
Fagron	Frutose	18082005	1
Fagron	Frutose	181018-01	1
Fagron	Frutose	1910020-01	1
Fagron	Frutose	19C19-B02-361846	1
Fagron	Frutose	3014Q-03394	1
Fagron	Frutose	326259	1
Fagron	Frutose	508Q-03394	1
Fagron	Frutose	516Q-03394	1
Fagron	Frutose	5217M-03394	1
Fagron	Frutose	7K21-N12	1
Fagron	Frutose	FR1413072	1
Fagron	Frutose	FR1443072	8
Fagron	Frutose	FR1713142	2
Fagron	Frutose	K43537721	2
Fargon	Frutose	14E01-B04-293506	2
Fargon	Frutose	15I21-B01-312701	1
Fiebig	Frutose	19169903	1
Finteler Apotheke	Frutose	16283910	1
fragon	Frutose	FR1413072	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gatt Koller	Frutose	1544/05141914	1
Gatt-Koller / Phoenix	Frutose	3156/0813	1
GEHE 17.06.2014	Frutose	13098913	1
Gehe	Frutose	1607030-01	2
Gehe	Frutose	17346404	1
GEHE	Frutose	1803040-01	2
Gehe	Frutose	18082005	1
Gehe	Frutose	1906017-01	1
Gehe	Frutose	2006019-01	1
gehe	Frutose	210200802	1
Gehe	Frutose	22003150021	2
gehe	Frutose	2203030-01	2
Gehe	Frutose	23003367001	1
geibo	Frutose	192965002	4
Geilenkirchen	Frutose	17007707	1
Geilenkirchen	Frutose	17143904	1
Geilenkirchen	Frutose	18082012	1
Geilenkirchen	Frutose	180822	1
Geilenkirchen	Frutose	18291613	7
Geilenkirchen	Frutose	19169904	2
Jenne	Frutose	14A16-B07	1
Jenne	Frutose	15A16-B07	1
JENNE	Frutose	17L22-B02	2
Lihn/Reformhaus	Frutose	713E-03394	2
Nachprüfung	Frutose	1906017-01	1
Noweda	Frutose	1205022-01	1
Noweda	Frutose	16283910	1
Noweda	Frutose	1710034-01	4
Noweda	Frutose	17143902	1
Noweda	Frutose	1906017-01	2
Noweda	Frutose	1910020-01	2
Noweda	Frutose	19169903	1
Noweda	Frutose	20003599001	1
Noweda	Frutose	2003150015	1
Noweda	Frutose	2203030-02	1
Noweda	Frutose	FS2P00251808-502	1
Phoenix 05.08.2014	Frutose	FR1336122	3
Phoenix 11.12.2018	Frutose	1803040-01	1
Phoenix 17.11.19	Frutose	1803044-01	1
Phoenix 22.12.14	Frutose	1307022-01	1
Phoenix 22.12.14	Frutose	1401004-01	1
Phoenix	Frutose	15I21-B01	1
phoenix	Frutose	1906017-01	1
Phoenix	Frutose	1906017-01	1
Phoenix	Frutose	21000686015	1
Phönisx	Frutose	18291602	1
Phönix 17.05.2019	Frutose	1811018-01	2
Phönix Euro	Frutose	FS2P00251707-304	1
Phönix	Frutose	12K28-N06	1
PHÖNIX	Frutose	1710034-01	1
PHÖNIX	Frutose	17L22-B02-346104	1
Sanacorp	Frutose	17346404	1
SANACORP	Frutose	1811018-01	2
Sanacorp	Frutose	2212011-01	3
Sanacorp	Frutose	K43537721	1
Synopharm	Frutose	202A052	1

- 234 799 spectra from 1515 *Apo-Ident* customers from a total of 48 971 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Frutose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Frutose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	921	0	201 163
Type C	0	1267	1	234 799

The substance/substance group *Frutose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3485 %)
Type C	100.0000 % (> 99.9007 %)	99.9211 % (> 99.6845 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21281	22481	11,28	93,87
21934	21934	0,00	90,26
22292	22292	0,00	90,08
22481	22481	0,00	91,42
22490	22292	5,26	91,22
22986	22986	0,00	89,52
23018	22292	5,74	90,82
23082	22481	7,11	91,25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fumarato de quetiapina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005949-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fumarato de quetiapina; Quetiapina, fumarato; Quetiapini fumaras

Special notes

When selecting the *Fumarato de quetiapina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fumarato de quetiapina	2	1	0

Second-stage model

For differentiation of the substance/substance group *Fumarato de quetiapina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fumarato de quetiapina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	147,37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fumarato de quetiapina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fumarato de quetiapina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Hetero Dru…	Fumarato de quetiapina	QU22040055	26402	40	20220510
ZCL Chemic…	Fumarato de quetiapina	QTP4206421	25834	50	2301088

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 90 spectra of 2 reference samples from the substance/substance group *Fumarato de quetiapina*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 872 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 4 reference samples from the substance/substance group *Fumarato de quetiapina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
ZCL Chemicals Ltd.	Fumarato de quetiapina	QTP4214921	25899	50
Hetero Drugs Ltd.	Fumarato de quetiapina	QU22040055	26402SI†	20
ZCL Chemicals Ltd.	Fumarato de quetiapina	QTP4206421	25834SI†	10
ZCL Chemicals Ltd.	Fumarato de quetiapina	QTP4214921	25899SI	10

- 201 994 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Fumarato de quetiapina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fumarato de quetiapina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fumarato de quetiapina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	90	0	152 872
Type B	0	77	13	201 994
Type C	0	0	0	236 067

The substance/substance group *Fumarato de quetiapina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 93.3333 %)
Type B	100.0000 % (> 99.9912 %)	85.5556 % (> 82.2222 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25834	25834	0,00	222,64
26402	25834	19,08	233,49

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Furoato de mometasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20100-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Furoato de mometasona; Mometasona, furoato; Mometasoni furoas

Special notes

When selecting the *Furoato de mometasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Furoato de mometasona	8	12	479

Second-stage model

For differentiation of the substance/substance group *Furoato de mometasona* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Furoato de mometasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de naloxona di-hidratado	121,87	–
⋮	⋮	⋮
Sulfato de atropina	>50	50,45
Sorbato de potássio	>50	112,83
Citrato monobásico de magnésio, hid…	>50	130,56
Hidrocortisona	>50	173,97
Quinolina amarela	>50	262,50
Escina, hidrossolúvel	>50	299,27
Cloridrato de propranolol	>50	310,00
Sacarina sódica	>50	405,28
Orotato de cálcio di-hidratado	>50	524,82
Fenitoína	>50	529,64

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Furoato de mometasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Furoato de mometasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Furoato de mometasona	160286	22433	60	20160316*
Caelo	Furoato de mometasona	163532	23046	40	20170104*
Euro OTC	Furoato de mometasona	1403015-01	21602	60	20140503
Euro OTC	Furoato de mometasona	1403015-01	21602SI	31	20140503
Euro OTC	Furoato de mometasona	1510036	22238	60	20151118*
Euro OTC	Furoato de mometasona	1510036	22238SI	30	20151118*
Euro OTC	Furoato de mometasona	1610009	23136	40	20170321*
Euro OTC	Furoato de mometasona	2305005	26766	40	20230630*
Euro OTC	Furoato de mometasona	2305005	26766SI	30	20230630*
Fagron	Furoato de mometasona	13F17-N01	20850	40	20130620

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Furoato de mometasona	13F17-N01	20850SI	44	20130620
Fagron	Furoato de mometasona	16A20-B06-319750	22887	40	20160209
Fagron	Furoato de mometasona	16A20-B06-319750	22887SI	30	20160209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 545 spectra of 13 reference samples from the substance/substance group *Furoato de mometasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 417 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 904 spectra of 27 reference samples from the substance/substance group *Furoato de mometasona*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Furoato de mometasona	13304605	21374	60
Caelo	Furoato de mometasona	183341	24563	40
Caelo	Furoato de mometasona	23001247	27248	40
Euro OTC	Furoato de mometasona	1606021	22715	40
Euro OTC	Furoato de mometasona	1711027	23878	40
Euro OTC	Furoato de mometasona	1810008	24295	40
Euro OTC	Furoato de mometasona	1906035	24794	40
Euro OTC	Furoato de mometasona	2001040	25159	40
Euro OTC	Furoato de mometasona	2003056	25167	40
Euro OTC	Furoato de mometasona	2008002	25408	40
Euro OTC	Furoato de mometasona	2106014	25869	50
Fagron	Furoato de mometasona	22C15-B06-221102	26295	35

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Furoato de mometasona	13304605	21374SI	38
Caelo	Furoato de mometasona	160286	22433SI†	30
Caelo	Furoato de mometasona	163532	23046SI†	23
Caelo	Furoato de mometasona	183341	24563SI	21
Caelo	Furoato de mometasona	23001247	27248SI	30
Euro OTC	Furoato de mometasona	1606021	22715SI	33
Euro OTC	Furoato de mometasona	1610009	23136SI†	20
Euro OTC	Furoato de mometasona	1711027	23878SI	27
Euro OTC	Furoato de mometasona	1810008	24295SI	20
Euro OTC	Furoato de mometasona	1906035	24794SI	24
Euro OTC	Furoato de mometasona	2001040	25159SI	30
Euro OTC	Furoato de mometasona	2003056	25167SI	22
Euro OTC	Furoato de mometasona	2008002	25408SI	20
Euro OTC	Furoato de mometasona	2106014	25869SI	31
Fagron	Furoato de mometasona	22C15-B06-221102	26295SI	30

- 201 180 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2733 spectra from 769 *Apo-Ident* customers from 514 batches from the substance/substance group *Furoato de mometasona*.
- Among them are spectra of independent samples from 478 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Furoato de mometasona	20003486021	1
	Furoato de mometasona	20003486024	4
	Furoato de mometasona	20003486026	1
	Furoato de mometasona	20003486027	1
	Furoato de mometasona	20003486029	3
	Furoato de mometasona	20003486030	4
	Furoato de mometasona	20003486034	8
	Furoato de mometasona	20003486035	8
	Furoato de mometasona	20G24-B03-1968709	1
	Furoato de mometasona	20G24-B03-197086	1
	Furoato de mometasona	2106014-01	16
	Furoato de mometasona	21B26-B05-203100	7
	Furoato de mometasona	21B26-B05-2031000	1
	Furoato de mometasona	22C15-B06-221102	1
	Furoato de mometasona	22C15-B06-223109	1
	Furoato de mometasona	22C15-B06-223110	1
	Furoato de mometasona	22C15-B06-227594	3
	Furoato de mometasona	23001247005	3
	Furoato de mometasona	23001247006	3
	Furoato de mometasona	2305005-01	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Furoato de mometasona	24D10-B13-236853	1
	Furoato de mometasona	B02-2346500	1
	Furoato de mometasona	B03-1970806	2
AARTI / Gehe	Furoato de mometasona	20000787001	1
AARTI Industries/Phoenix	Furoato de mometasona	MF-18013(JM-01)-001	1
AARTI Industries/Phoenix	Furoato de mometasona	MF-20002(JM-01)-001	1
Ador Pharma	Furoato de mometasona	APMOM006/0517M	1
AEP	Furoato de mometasona	20003486012	1
AHD 20.06.14 EK 37,29	Furoato de mometasona	12C07-B05-291268	1
AHD/EuRho	Furoato de mometasona	2001040-01	1
Alliance Health 27.0...	Furoato de mometasona	13J23-N02	1
Alliance Healthcare	Furoato de mometasona	B03-1968709	2
Alte Apotheke	Furoato de mometasona	1606021-01	1
Anzag	Furoato de mometasona	12J29N03	1
Anzag	Furoato de mometasona	13D08-N06	1
Audor Pharma	Furoato de mometasona	APMOM006/0117M	4
Audor Pharma	Furoato de mometasona	APMOM006/0177M	1
Audor Pharma	Furoato de mometasona	APMOM006/0517M	7
Audor Pharma	Furoato de mometasona	APMOM010/0116M	3
Audor Pharma	Furoato de mometasona	APMOM301/0118-1M	2
Audor Pharma	Furoato de mometasona	APMOM301/0118-8M	1
Audor Pharma	Furoato de mometasona	APMOM301/0118M	3
Beiersdorf	Furoato de mometasona	18026011	1
Bombastus	Furoato de mometasona	16J24-B11-335793	1
Bombastus	Furoato de mometasona	18B19-B07-352632	1
Cael Sanacorp 05.02.2016	Furoato de mometasona	14H06-B07-298481	1
Caelo	Furoato de mometasona		1
Caelo	Furoato de mometasona	116181714	1
Caelo	Furoato de mometasona	12035601	1
Caelo	Furoato de mometasona	12035607	2
Caelo	Furoato de mometasona	12035608	2
Caelo	Furoato de mometasona	12339604	1
Caelo	Furoato de mometasona	12351202	1
Caelo	Furoato de mometasona	12351205	2
Caelo	Furoato de mometasona	12351207	1
Caelo	Furoato de mometasona	12351208	1
Caelo	Furoato de mometasona	12351210	1
Caelo	Furoato de mometasona	12351215	4
Caelo	Furoato de mometasona	13304603	1
Caelo	Furoato de mometasona	13304604	2
Caelo	Furoato de mometasona	13304605	4
Caelo	Furoato de mometasona	13304606	4
Caelo	Furoato de mometasona	13304609	1
Caelo	Furoato de mometasona	13304612	1
Caelo	Furoato de mometasona	13304614	1
Caelo	Furoato de mometasona	13F27-N02	1
Caelo	Furoato de mometasona	13H13N04	1
Caelo	Furoato de mometasona	13H13-N04	1
Caelo	Furoato de mometasona	13J23-N02	1
Caelo	Furoato de mometasona	14281101	2
Caelo	Furoato de mometasona	14281102	4
Caelo	Furoato de mometasona	14281103	2
Caelo	Furoato de mometasona	14C07-B05-291268	8
Caelo	Furoato de mometasona	14E20-B04	1
Caelo	Furoato de mometasona	14e20-b04-291267	1
Caelo	Furoato de mometasona	14E20-B04-291267	1
Caelo	Furoato de mometasona	14H06-B07298481	1
Caelo	Furoato de mometasona	15/11-B02-314479	1
Caelo	Furoato de mometasona	15/11-Bo2-314479	1
Caelo	Furoato de mometasona	1510036-001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Furoato de mometasona	151003601	1
Caelo	Furoato de mometasona	1510036-02	2
Caelo	Furoato de mometasona	15110301	4
Caelo	Furoato de mometasona	15110305	4
Caelo	Furoato de mometasona	15189801	3
Caelo	Furoato de mometasona	15189802	5
Caelo	Furoato de mometasona	15189804	3
Caelo	Furoato de mometasona	15189806	1
Caelo	Furoato de mometasona	15189807	5
Caelo	Furoato de mometasona	15189809	5
Caelo	Furoato de mometasona	15279003	1
Caelo	Furoato de mometasona	15279004	6
Caelo	Furoato de mometasona	15b11b03	1
Caelo	Furoato de mometasona	15B11-B03-304121	2
Caelo	Furoato de mometasona	15B11B03304122	1
Caelo	Furoato de mometasona	15G08-B11-310864	2
Caelo	Furoato de mometasona	15G08-B11-310865	1
Caelo	Furoato de mometasona	15G08-B11-317182	1
Caelo	Furoato de mometasona	15G08-B11-322739	1
Caelo	Furoato de mometasona	1602809	1
Caelo	Furoato de mometasona	16028601	4
Caelo	Furoato de mometasona	16028602	7
Caelo	Furoato de mometasona	16028604	6
Caelo	Furoato de mometasona	16028605	2
Caelo	Furoato de mometasona	16028606	7
Caelo	Furoato de mometasona	16028607	8
Caelo	Furoato de mometasona	16028609	9
Caelo	Furoato de mometasona	1606021-01	6
Caelo	Furoato de mometasona	1610009-01	8
Caelo	Furoato de mometasona	16181703	1
Caelo	Furoato de mometasona	16181704	8
Caelo	Furoato de mometasona	16181705	4
Caelo	Furoato de mometasona	16181708	4
Caelo	Furoato de mometasona	16181709	6
Caelo	Furoato de mometasona	16181710	5
Caelo	Furoato de mometasona	16181714	1
Caelo	Furoato de mometasona	16181715	7
Caelo	Furoato de mometasona	1635206	1
Caelo	Furoato de mometasona	1635209	1
Caelo	Furoato de mometasona	1635211	1
Caelo	Furoato de mometasona	16353201	7
Caelo	Furoato de mometasona	16353204	2
Caelo	Furoato de mometasona	16353205	4
Caelo	Furoato de mometasona	16353206	14
Caelo	Furoato de mometasona	16353207	15
Caelo	Furoato de mometasona	16353208	5
Caelo	Furoato de mometasona	16353209	20
Caelo	Furoato de mometasona	16353210	4
Caelo	Furoato de mometasona	16353211	14
Caelo	Furoato de mometasona	16353212	2
Caelo	Furoato de mometasona	1653205	1
Caelo	Furoato de mometasona	16A20-B06-319748	1
Caelo	Furoato de mometasona	16A20-B06-319749	1
Caelo	Furoato de mometasona	16C24_B03_324852	2
Caelo	Furoato de mometasona	16C24-B03-324852	1
Caelo	Furoato de mometasona	16C24-B03-327346	1
Caelo	Furoato de mometasona	16C24-B03-328272	1
Caelo	Furoato de mometasona	16J24-B11	1
Caelo	Furoato de mometasona	16J24-B11-332112	1
Caelo	Furoato de mometasona	16J24B11-334371	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Furoato de mometasona	16J24-B11-334371	2
Caelo	Furoato de mometasona	16J24-B11-335793	1
Caelo	Furoato de mometasona	1704012A	1
Caelo	Furoato de mometasona	1711027	1
Caelo	Furoato de mometasona	1711027-01	1
Caelo	Furoato de mometasona	17348901	10
Caelo	Furoato de mometasona	17D19-B02	3
Caelo	Furoato de mometasona	17D19-B02-339277	1
Caelo	Furoato de mometasona	17D19-B02-342643	3
Caelo	Furoato de mometasona	17D19-B02-34476	1
Caelo	Furoato de mometasona	17D19-B02-347348	2
Caelo	Furoato de mometasona	17D1-B02-344776	1
Caelo	Furoato de mometasona	18026001	24
Caelo	Furoato de mometasona	18026002	1
Caelo	Furoato de mometasona	18026003	5
Caelo	Furoato de mometasona	18026004	16
Caelo	Furoato de mometasona	18026005	1
Caelo	Furoato de mometasona	18026006	6
Caelo	Furoato de mometasona	18026007	9
Caelo	Furoato de mometasona	18026008	5
Caelo	Furoato de mometasona	18026009	3
Caelo	Furoato de mometasona	18026010	1
Caelo	Furoato de mometasona	18026011	23
Caelo	Furoato de mometasona	18026012	14
Caelo	Furoato de mometasona	18026015	6
Caelo	Furoato de mometasona	18026017	6
Caelo	Furoato de mometasona	1802603	1
Caelo	Furoato de mometasona	1802611	1
Caelo	Furoato de mometasona	1806012	1
Caelo	Furoato de mometasona	1810008-01	2
Caelo	Furoato de mometasona	18102013B	1
Caelo	Furoato de mometasona	18334101	9
Caelo	Furoato de mometasona	18334102	19
Caelo	Furoato de mometasona	18334103	1
Caelo	Furoato de mometasona	18334104	20
Caelo	Furoato de mometasona	18334106	12
Caelo	Furoato de mometasona	18334108	9
Caelo	Furoato de mometasona	18334109P-191111-4	1
Caelo	Furoato de mometasona	18334110	13
Caelo	Furoato de mometasona	18B19B07-351001	1
Caelo	Furoato de mometasona	18B19-B07-351351	1
Caelo	Furoato de mometasona	18B19-B07-352632	1
Caelo	Furoato de mometasona	18B19-B07-354319	1
Caelo	Furoato de mometasona	18B-B07-354320	1
Caelo	Furoato de mometasona	192006004	7
Caelo	Furoato de mometasona	19200601	21
Caelo	Furoato de mometasona	19200602	19
Caelo	Furoato de mometasona	19200603	14
Caelo	Furoato de mometasona	19200604	5
Caelo	Furoato de mometasona	19200605	9
Caelo	Furoato de mometasona	19F13-B12-191761	1
Caelo	Furoato de mometasona	200000787008	1
Caelo	Furoato de mometasona	200003486010	1
Caelo	Furoato de mometasona	2000078004	1
Caelo	Furoato de mometasona	20000787001	21
Caelo	Furoato de mometasona	20000787002	1
Caelo	Furoato de mometasona	20000787004	17
Caelo	Furoato de mometasona	20000787005	20
Caelo	Furoato de mometasona	20000787007	12
Caelo	Furoato de mometasona	20000787008	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Furoato de mometasona	20000787009	1
Caelo	Furoato de mometasona	20000787010	9
Caelo	Furoato de mometasona	20000787012	15
Caelo	Furoato de mometasona	20000787013	8
Caelo	Furoato de mometasona	2000078787001	1
Caelo	Furoato de mometasona	2000346006	1
Caelo	Furoato de mometasona	20003486002	12
Caelo	Furoato de mometasona	20003486004	34
Caelo	Furoato de mometasona	20003486005	1
Caelo	Furoato de mometasona	20003486006	15
Caelo	Furoato de mometasona	20003486009	3
Caelo	Furoato de mometasona	20003486010	11
Caelo	Furoato de mometasona	20003486011	15
Caelo	Furoato de mometasona	20003486012	10
Caelo	Furoato de mometasona	20003486013	1
Caelo	Furoato de mometasona	20003486016	10
Caelo	Furoato de mometasona	20003486017	7
Caelo	Furoato de mometasona	20003486018	10
Caelo	Furoato de mometasona	20003486021	6
Caelo	Furoato de mometasona	20003486024	13
Caelo	Furoato de mometasona	20003486026	3
Caelo	Furoato de mometasona	20003486027	4
Caelo	Furoato de mometasona	20003486030	3
Caelo	Furoato de mometasona	20003486035	1
Caelo	Furoato de mometasona	20003486036	1
Caelo	Furoato de mometasona	200034866016	1
Caelo	Furoato de mometasona	200034896004	1
Caelo	Furoato de mometasona	2000787001	1
Caelo	Furoato de mometasona	2000787004	1
Caelo	Furoato de mometasona	2000787007	1
Caelo	Furoato de mometasona	2000787013	1
Caelo	Furoato de mometasona	200315A	1
Caelo	Furoato de mometasona	2003486026	1
Caelo	Furoato de mometasona	20g24-b03-196879	1
Caelo	Furoato de mometasona	20G24-B03-196879	1
Caelo	Furoato de mometasona	220003486026	1
Caelo	Furoato de mometasona	240913a	1
Caelo	Furoato de mometasona	2885	1
Caelo	Furoato de mometasona	34860062	1
Caelo	Furoato de mometasona	701834-0002	1
Caelo	Furoato de mometasona	9530001	1
Caelo	Furoato de mometasona	9530018	1
Caelo	Furoato de mometasona	APMOM006/0117M	1
Caelo	Furoato de mometasona	MOM001/0317	1
Caelo	Furoato de mometasona	MOM010/0116	3
Caelo	Furoato de mometasona	NO1352M	1
Caelo	Furoato de mometasona	NT1568M	1
Caelo	Furoato de mometasona	NU0698M	1
Caelo	Furoato de mometasona	NV1000M	1
Caeo/Noweda	Furoato de mometasona	15279003	1
Caeo	Furoato de mometasona	12351201	1
Caeolo/Gehe	Furoato de mometasona	16J24-B11-332112	1
Caeolo/Gehe	Furoato de mometasona	18334104	1
Caesa / Alliance Hea…	Furoato de mometasona	18026012	1
Caesar & Lorenz GmbH	Furoato de mometasona	18334108	1
Caesar & Lorenz GmbH	Furoato de mometasona	20000787001	1
Caesar & Loretz GmbH…	Furoato de mometasona	2000078005	1
Caesar & Loretz GmbH…	Furoato de mometasona	18026015	1
Caesar & Loretz GmbH…	Furoato de mometasona	20000787005	1
Caesar & Loretz GmbH…	Furoato de mometasona	11H10-N04	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/ AHD	Furoato de mometasona	20003486016	1
Caesar & Loretz GmbH…	Furoato de mometasona	20000787005	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486017	2
Caesar & Loretz GmbH…	Furoato de mometasona	20003486010	1
Caesar & Loretz GmbH/AHD	Furoato de mometasona	20003486006	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486006	2
Caesar & Loretz GmbH…	Furoato de mometasona	20003486021	1
Caesar & Loretz GmbH/Gehe	Furoato de mometasona	19200605	1
Caesar & Loretz GmbH/Gehe	Furoato de mometasona	20003486016	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486004	4
Caesar & Loretz GmbH…	Furoato de mometasona	18334108	1
Caesar & Loretz GmbH…	Furoato de mometasona	20000787001	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486026	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486034	1
Caesar & Loretz GmbH…	Furoato de mometasona	20000787001	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486024	1
Caesar & Loretz GmbH/Otto	Furoato de mometasona	20000787010	1
Caesar & Loretz GmbH/Ph	Furoato de mometasona	20003486018	1
Caesar & Loretz GmbH…	Furoato de mometasona	2000078712	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486002	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486004	1
Caesar & Loretz GmbH…	Furoato de mometasona	20000787008	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486011	1
Caesar & Loretz GmbH/S	Furoato de mometasona	20003486010	1
Caesar & Loretz GmbH/S	Furoato de mometasona	20003486024	1
Caesar & Loretz GmbH/Sa	Furoato de mometasona	18334108	1
Caesar & Loretz GmbH/Sa	Furoato de mometasona	19200601	1
Caesar & Loretz GmbH/Sana	Furoato de mometasona	20003486012	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486010	1
Caesar & Loretz GmbH…	Furoato de mometasona	20003486018	2
Caesar & Loretz GmbH…	Furoato de mometasona	20003486024	1
Caesar & Loretz GmbH	Furoato de mometasona	12035601	1
Caesar & Loretz GmbH	Furoato de mometasona	16028609	2
Caesar & Loretz GmbH	Furoato de mometasona	18026001	1
Caesar & Loretz GmbH	Furoato de mometasona	18026012	5
Caesar & Loretz GmbH	Furoato de mometasona	18026013	1
Caesar & Loretz GmbH	Furoato de mometasona	18026014	1
Caesar & Loretz GmbH	Furoato de mometasona	18026017	1
Caesar & Loretz GmbH	Furoato de mometasona	18072120	1
Caesar & Loretz GmbH	Furoato de mometasona	18334101	4
Caesar & Loretz GmbH	Furoato de mometasona	18334102	3
Caesar & Loretz GmbH	Furoato de mometasona	18334104	4
Caesar & Loretz GmbH	Furoato de mometasona	18334106	2
Caesar & Loretz GmbH	Furoato de mometasona	18334108	8
Caesar & Loretz GmbH	Furoato de mometasona	18334110	3
Caesar & Loretz GmbH	Furoato de mometasona	19200601	4
Caesar & Loretz GmbH	Furoato de mometasona	19200602	2
Caesar & Loretz GmbH	Furoato de mometasona	19200603	2
Caesar & Loretz GmbH	Furoato de mometasona	19200604	1
Caesar & Loretz GmbH	Furoato de mometasona	19200605	7
Caesar & Loretz GmbH	Furoato de mometasona	200003486024	1
Caesar & Loretz GmbH	Furoato de mometasona	20000787001	8
Caesar & Loretz GmbH	Furoato de mometasona	20000787002	1
Caesar & Loretz GmbH	Furoato de mometasona	20000787004	2
Caesar & Loretz GmbH	Furoato de mometasona	20000787005	4
Caesar & Loretz GmbH	Furoato de mometasona	20000787007	3
Caesar & Loretz GmbH	Furoato de mometasona	20000787008	2
Caesar & Loretz GmbH	Furoato de mometasona	20000787010	4
Caesar & Loretz GmbH	Furoato de mometasona	20000787012	2
Caesar & Loretz GmbH	Furoato de mometasona	20000787013	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Furoato de mometasona	20003486002	11
Caesar & Loretz GmbH	Furoato de mometasona	20003486004	14
Caesar & Loretz GmbH	Furoato de mometasona	20003486006	8
Caesar & Loretz GmbH	Furoato de mometasona	20003486008	4
Caesar & Loretz GmbH	Furoato de mometasona	20003486010	1
Caesar & Loretz GmbH	Furoato de mometasona	20003486011	11
Caesar & Loretz GmbH	Furoato de mometasona	20003486012	3
Caesar & Loretz GmbH	Furoato de mometasona	20003486016	3
Caesar & Loretz GmbH	Furoato de mometasona	20003486017	5
Caesar & Loretz GmbH	Furoato de mometasona	20003486018	8
Caesar & Loretz GmbH	Furoato de mometasona	20003486020	1
Caesar & Loretz GmbH	Furoato de mometasona	20003486021	12
Caesar & Loretz GmbH	Furoato de mometasona	20003486024	2
Caesar & Loretz GmbH	Furoato de mometasona	20003486026	2
Caesar & Loretz GmbH	Furoato de mometasona	20003486027	2
Caesar & Loretz GmbH	Furoato de mometasona	2001040-01	2
Caesar & Loretz GmbH	Furoato de mometasona	22C15-B06-221102	1
Caesar & Loretz GmbH	Furoato de mometasona	30000787007	1
Caesar & Loretz GmbH	Furoato de mometasona	B03-1968709	1
Caesar & Loretz GmbH	Furoato de mometasona	B03-1970806	1
Caesar & Loretz Hilden	Furoato de mometasona	18026012	1
Caesar & Loretz/Geil...	Furoato de mometasona	20003486006	2
Caesar & Loretz/Noweda	Furoato de mometasona	18026012	1
Caesar u Loretz	Furoato de mometasona	15279004	2
Caesar u. Loretz GmbH	Furoato de mometasona	19200605	1
Caesar und Loretz GmbH	Furoato de mometasona	2000787010	1
caesar&Loretz GmbH,P...	Furoato de mometasona	16028604	1
Caesar&loretz,AHC,08...	Furoato de mometasona		1
Calo/AHD	Furoato de mometasona	19200603	1
Carlo/Phönix/21,89	Furoato de mometasona	18334102	1
Cealo/Anzag	Furoato de mometasona	18026012	1
Cealo	Furoato de mometasona	20003486004	2
EuRho / 2	Furoato de mometasona	1906035-01	1
EuRho / 2	Furoato de mometasona	2003056-01	1
EuRho / Noweda	Furoato de mometasona	1906035-01	2
EuRho/AHD	Furoato de mometasona	2003056-01	1
EuRho/AHD	Furoato de mometasona	2008002-01	3
EuRho/Gehe	Furoato de mometasona	2001040-01	1
EuRho/Gehe	Furoato de mometasona	2106014-01	1
EuRho/Ph	Furoato de mometasona	2001040-01	2
EuRho/Phönix	Furoato de mometasona	1307037-01	2
EuRho	Furoato de mometasona	1408010-01	1
EuRho	Furoato de mometasona	15/11-B02-315705	1
Eurho	Furoato de mometasona	18B19-B07-352744	1
EuRho	Furoato de mometasona	2003056-01	1
EuRho	Furoato de mometasona	2008002-01	1
Euro OTC	Furoato de mometasona		2
Euro OTC	Furoato de mometasona	1203024-02	1
Euro OTC	Furoato de mometasona	1307037-01	1
Euro OTC	Furoato de mometasona	1408010-01	2
Euro OTC	Furoato de mometasona	1504012-01	7
Euro OTC	Furoato de mometasona	1504012-02	5
Euro OTC	Furoato de mometasona	1510036-01	15
Euro OTC	Furoato de mometasona	15G08-B11-317182	1
Euro OTC	Furoato de mometasona	15G08-B11-322738	2
Euro OTC	Furoato de mometasona	160009-01	1
Euro OTC	Furoato de mometasona	160602101	1
Euro OTC	Furoato de mometasona	1606021-01	8
Euro OTC	Furoato de mometasona	16100009-01	3
Euro OTC	Furoato de mometasona	1610009-001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Furoato de mometasona	161000901	1
Euro OTC	Furoato de mometasona	1610009-01	27
Euro OTC	Furoato de mometasona	16J24-b11	1
Euro OTC	Furoato de mometasona	16j24-B11-332111	1
Euro OTC	Furoato de mometasona	1711027	1
Euro OTC	Furoato de mometasona	171102701	1
Euro OTC	Furoato de mometasona	1711027-01	9
Euro OTC	Furoato de mometasona	1711027-02	4
Euro OTC	Furoato de mometasona	17D19-B02-342643	1
Euro OTC	Furoato de mometasona	17D19B02347349	1
Euro OTC	Furoato de mometasona	18026006	1
Euro OTC	Furoato de mometasona	1810002-01	1
Euro OTC	Furoato de mometasona	1810008_01	1
Euro OTC	Furoato de mometasona	181000801	2
Euro OTC	Furoato de mometasona	1810008-01	28
Euro OTC	Furoato de mometasona	1810008-01P-200331-2	1
Euro OTC	Furoato de mometasona	18334108	1
Euro OTC	Furoato de mometasona	18B19-B07-352632	1
Euro OTC	Furoato de mometasona	19060035	1
Euro OTC	Furoato de mometasona	1906035	2
Euro OTC	Furoato de mometasona	190603501	2
Euro OTC	Furoato de mometasona	1906035-01	31
Euro OTC	Furoato de mometasona	20008002-01	1
Euro OTC	Furoato de mometasona	2001040-01	15
Euro OTC	Furoato de mometasona	2003056-01	45
Euro OTC	Furoato de mometasona	200800-01	1
Euro OTC	Furoato de mometasona	200800201	4
Euro OTC	Furoato de mometasona	2008002-01	86
Euro OTC	Furoato de mometasona	2106014-01	30
Euro OTC	Furoato de mometasona	23051822	1
Euro OTC	Furoato de mometasona	5991	1
Euro OTC	Furoato de mometasona	83919-23-7	1
Euro OTG	Furoato de mometasona	1403015-01	1
EURO/Noweda	Furoato de mometasona	2003056-01	1
EuRoh/ Gehe	Furoato de mometasona	2008002-01	1
Fagr/sana EK: EUR 39,2...	Furoato de mometasona	18B19-B07-35151	1
Fagro/Noweda	Furoato de mometasona	17D19-B02-339277	1
Fagro	Furoato de mometasona	1511B02	1
Fagron	Furoato de mometasona		1
Fagron	Furoato de mometasona	10805-N12	1
Fagron	Furoato de mometasona	10C29-N10	1
Fagron	Furoato de mometasona	10E31-N26	1
Fagron	Furoato de mometasona	11C02-N03	2
Fagron	Furoato de mometasona	11F08-N03	1
Fagron	Furoato de mometasona	11H10-N01	1
Fagron	Furoato de mometasona	11h10-n04	1
Fagron	Furoato de mometasona	11H10-N04	2
Fagron	Furoato de mometasona	11K28-N09	2
Fagron	Furoato de mometasona	12B22-N01	1
Fagron	Furoato de mometasona	12B22-N04	1
Fagron	Furoato de mometasona	12e02-n11	1
Fagron	Furoato de mometasona	12E02-N11	4
Fagron	Furoato de mometasona	12H09-N02	7
Fagron	Furoato de mometasona	12I29-N03	1
Fagron	Furoato de mometasona	12J29-N01	1
Fagron	Furoato de mometasona	12J29-N03	4
Fagron	Furoato de mometasona	13d08-n06	1
Fagron	Furoato de mometasona	13D08N06	1
Fagron	Furoato de mometasona	13D08-N06	14
Fagron	Furoato de mometasona	13Do8-NO6	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Furoato de mometasona	13f17-n01	1
Fagron	Furoato de mometasona	13F17-N01	9
Fagron	Furoato de mometasona	13F27-N02	7
Fagron	Furoato de mometasona	13F27-NO2	1
Fagron	Furoato de mometasona	13F7-N01	1
Fagron	Furoato de mometasona	13H13-N04	10
Fagron	Furoato de mometasona	13H13-NO4	1
Fagron	Furoato de mometasona	13j23_n02	1
Fagron	Furoato de mometasona	13j23-N02	1
Fagron	Furoato de mometasona	13J23-N02	21
Fagron	Furoato de mometasona	13j23-no2	1
Fagron	Furoato de mometasona	140305MF	1
Fagron	Furoato de mometasona	14C07-B05-291264	1
Fagron	Furoato de mometasona	14C07-B05-291266	2
Fagron	Furoato de mometasona	14C07-B05-291268	5
Fagron	Furoato de mometasona	14E20-B04	4
Fagron	Furoato de mometasona	14e20b04291265	1
Fagron	Furoato de mometasona	14e20-b04-291265	1
Fagron	Furoato de mometasona	14E20-B04-291265	3
Fagron	Furoato de mometasona	14e20-b04-291267	1
Fagron	Furoato de mometasona	14E20-B04-291267	7
Fagron	Furoato de mometasona	14E20-B04-291269	2
Fagron	Furoato de mometasona	14E20-B04-291271	1
Fagron	Furoato de mometasona	14E20-B04-294645	7
Fagron	Furoato de mometasona	14E20-B04-302374	2
Fagron	Furoato de mometasona	14H06-B07297240	1
Fagron	Furoato de mometasona	14H06-B07-297240	3
Fagron	Furoato de mometasona	14H06-B07-298481	2
Fagron	Furoato de mometasona	14H06-B07-298482	7
Fagron	Furoato de mometasona	14H06-B07-302375	2
Fagron	Furoato de mometasona	14H06-B07-302376	3
Fagron	Furoato de mometasona	15/11-B02	4
Fagron	Furoato de mometasona	15/11-B02-314479	5
Fagron	Furoato de mometasona	15/11B02315705	2
Fagron	Furoato de mometasona	15/11-B02-315705	3
Fagron	Furoato de mometasona	15/11-B02-316705	1
Fagron	Furoato de mometasona	15B11-B03	2
Fagron	Furoato de mometasona	15b11-b03-304120	1
Fagron	Furoato de mometasona	15B11-B03-304120	7
Fagron	Furoato de mometasona	15B11B03304121	1
Fagron	Furoato de mometasona	15B11-B03-304121	9
Fagron	Furoato de mometasona	15B11B03304122	1
Fagron	Furoato de mometasona	15B11-B03-304122	6
Fagron	Furoato de mometasona	15B11-B03-304123	14
Fagron	Furoato de mometasona	15b11-b03-304124	1
Fagron	Furoato de mometasona	15B11-B03-304124	2
Fagron	Furoato de mometasona	15b11-b03-308276	2
Fagron	Furoato de mometasona	15B11-B03-308276	3
Fagron	Furoato de mometasona	15B11B03308860	1
Fagron	Furoato de mometasona	15B11-B03-308860	2
Fagron	Furoato de mometasona	15G08	1
Fagron	Furoato de mometasona	15G08-B11	3
Fagron	Furoato de mometasona	15G08-B11-0002	1
Fagron	Furoato de mometasona	15G08-B11-310864	8
Fagron	Furoato de mometasona	15G08-B11-312233	4
Fagron	Furoato de mometasona	15G08-B11-317182	9
Fagron	Furoato de mometasona	15G08-B11-322737	2
Fagron	Furoato de mometasona	15g08-b11-322738	1
Fagron	Furoato de mometasona	15G08B11322738	1
Fagron	Furoato de mometasona	15G08-B11-322738	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Furoato de mometasona	15G-B11-310864	1
Fagron	Furoato de mometasona	15I11-B02-314479	4
Fagron	Furoato de mometasona	15I11-B02-315705	1
Fagron	Furoato de mometasona	15J11-B02-315705	1
Fagron	Furoato de mometasona	16/24-B11-332122	1
Fagron	Furoato de mometasona	16181709	1
Fagron	Furoato de mometasona	16181714	1
Fagron	Furoato de mometasona	16724-B11-332112	1
Fagron	Furoato de mometasona	16A20-B06	3
Fagron	Furoato de mometasona	16A20-B06-319740	1
Fagron	Furoato de mometasona	16A20-B06-319748	7
Fagron	Furoato de mometasona	16A20-B06319749	1
Fagron	Furoato de mometasona	16A20-B06-319749	6
Fagron	Furoato de mometasona	16A20-B06-322739	6
Fagron	Furoato de mometasona	16A20-Bo6-319748	1
Fagron	Furoato de mometasona	16C24	1
Fagron	Furoato de mometasona	16C24-803-324851	1
Fagron	Furoato de mometasona	16C24B03	1
Fagron	Furoato de mometasona	16C24-B03	3
Fagron	Furoato de mometasona	16C24B03324851	1
Fagron	Furoato de mometasona	16C24-B03-324851	4
Fagron	Furoato de mometasona	16C24B03324852	1
Fagron	Furoato de mometasona	16C24-B03-324852	5
Fagron	Furoato de mometasona	16C24-B03-325575	1
Fagron	Furoato de mometasona	16C24-B03-326790	10
Fagron	Furoato de mometasona	16C24-B03-327346	4
Fagron	Furoato de mometasona	16c24-b03-327372	1
Fagron	Furoato de mometasona	16C24-b03-327372	1
Fagron	Furoato de mometasona	16C24-B03-327372	5
Fagron	Furoato de mometasona	16C24-B03-328272	6
Fagron	Furoato de mometasona	16J24-11-335793	1
Fagron	Furoato de mometasona	16j24-b11	1
Fagron	Furoato de mometasona	16J24-B11	6
Fagron	Furoato de mometasona	16j24-b11-329817	1
Fagron	Furoato de mometasona	16J24B11329817	1
Fagron	Furoato de mometasona	16J24-B11-329817	4
Fagron	Furoato de mometasona	16J24-B11-330978	5
Fagron	Furoato de mometasona	16J24-B11-332110	3
Fagron	Furoato de mometasona	16J24-B11-332111	5
Fagron	Furoato de mometasona	16J24B11332112	1
Fagron	Furoato de mometasona	16J24-B11-332112	14
Fagron	Furoato de mometasona	16J24B11334371	1
Fagron	Furoato de mometasona	16J24-B11-334371	9
Fagron	Furoato de mometasona	16j24-b11-335792	1
Fagron	Furoato de mometasona	16J24-B11-335792	1
Fagron	Furoato de mometasona	16j24b11335793	1
Fagron	Furoato de mometasona	16J24B11335793	1
Fagron	Furoato de mometasona	16J24-B11-335793	11
Fagron	Furoato de mometasona	17D1834	1
Fagron	Furoato de mometasona	17D19	1
Fagron	Furoato de mometasona	17D19_B02_339278	1
Fagron	Furoato de mometasona	17D19-B02	5
Fagron	Furoato de mometasona	17D19-B02_339278	1
Fagron	Furoato de mometasona	17D19-B02-33927	2
Fagron	Furoato de mometasona	17D19-B02-339276	3
Fagron	Furoato de mometasona	17D19B02339277	1
Fagron	Furoato de mometasona	17D19-B02339277	1
Fagron	Furoato de mometasona	17D19-B02-339277	4
Fagron	Furoato de mometasona	17D19-B02-339278	6
Fagron	Furoato de mometasona	17D19B02342642	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Furoato de mometasona	17D19-B02-342642	3
Fagron	Furoato de mometasona	17D19-B02-342643	20
Fagron	Furoato de mometasona	17D19-B02-344776	3
Fagron	Furoato de mometasona	17D19-B02-347347	5
Fagron	Furoato de mometasona	17D19-B02-347348	5
Fagron	Furoato de mometasona	17d19-b02-347349	1
Fagron	Furoato de mometasona	17D19B02347349	1
Fagron	Furoato de mometasona	17D19-B02-347349	15
Fagron	Furoato de mometasona	17D19-B02-3477347	1
Fagron	Furoato de mometasona	1814E3640	1
Fagron	Furoato de mometasona	18819-807	1
Fagron	Furoato de mometasona	18819-b07	1
Fagron	Furoato de mometasona	18819-B07-345319	1
Fagron	Furoato de mometasona	18819-B07-356278	1
Fagron	Furoato de mometasona	18819-B07-357640	3
Fagron	Furoato de mometasona	18B199-B07-354320	1
Fagron	Furoato de mometasona	18B19-B07	10
Fagron	Furoato de mometasona	18B19-B07-341351	1
Fagron	Furoato de mometasona	18b19-b07-351001	1
Fagron	Furoato de mometasona	18B19-B07-351001	1
Fagron	Furoato de mometasona	18B19-B07-351351	9
Fagron	Furoato de mometasona	18b19-b07-352632	1
Fagron	Furoato de mometasona	18B19B07352632	1
Fagron	Furoato de mometasona	18B19-B07-352632	17
Fagron	Furoato de mometasona	18B19-B07-352635	1
Fagron	Furoato de mometasona	18B19-B07-352744	9
Fagron	Furoato de mometasona	18B19B07352745	1
Fagron	Furoato de mometasona	18B19-B07-352745	13
Fagron	Furoato de mometasona	18B19-B07-354318	4
Fagron	Furoato de mometasona	18B19-B07-354319	5
Fagron	Furoato de mometasona	18B19-B07-354319MOM010/0118	1
Fagron	Furoato de mometasona	18B19-B07-354320	19
Fagron	Furoato de mometasona	18B19-B07-357228	3
Fagron	Furoato de mometasona	18B19-B07-357640	11
Fagron	Furoato de mometasona	191761	2
Fagron	Furoato de mometasona	19200604	1
Fagron	Furoato de mometasona	197086	1
Fagron	Furoato de mometasona	19F13B12191760	2
Fagron	Furoato de mometasona	19F13-B12-191760	5
Fagron	Furoato de mometasona	19F13B12191761	1
Fagron	Furoato de mometasona	19F13-B12-191761	22
Fagron	Furoato de mometasona	19F13-B12-1917610481	1
Fagron	Furoato de mometasona	19F13-B12-191762	8
Fagron	Furoato de mometasona	19F13-B191761	1
Fagron	Furoato de mometasona	20000787001	1
Fagron	Furoato de mometasona	20G24_B03-197086	1
Fagron	Furoato de mometasona	20G244-B03-196879	1
Fagron	Furoato de mometasona	20g24-803-196879	1
Fagron	Furoato de mometasona	20G24-B03	11
Fagron	Furoato de mometasona	20G24-B03-1968709	1
Fagron	Furoato de mometasona	20G24-B03-196879	27
Fagron	Furoato de mometasona	20G24B03197086	4
Fagron	Furoato de mometasona	20G24-B03-197086	23
Fagron	Furoato de mometasona	20G24-B03-201311	2
Fagron	Furoato de mometasona	20G24-B03-196879	2
Fagron	Furoato de mometasona	20G24-B03-201311	1
Fagron	Furoato de mometasona	210543	1
Fagron	Furoato de mometasona	2114M3640	1
Fagron	Furoato de mometasona	21B26-B05	2
Fagron	Furoato de mometasona	21b26-b05-203100	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Furoato de mometasona	21B26-B05-203100	22
Fagron	Furoato de mometasona	21B26-B05-203101	14
Fagron	Furoato de mometasona	21B26B05210542	1
Fagron	Furoato de mometasona	21B26-B05-210542	6
Fagron	Furoato de mometasona	21B26-B05-210543	7
Fagron	Furoato de mometasona	21B26-B05-213869	1
Fagron	Furoato de mometasona	21B26-B05-219115	1
Fagron	Furoato de mometasona	21B26-B05-219200	1
Fagron	Furoato de mometasona	21B26-BO5-213869	1
Fagron	Furoato de mometasona	2215I-07030	1
Fagron	Furoato de mometasona	22C15-B06-219423	2
Fagron	Furoato de mometasona	22C15B06221102	1
Fagron	Furoato de mometasona	22C15-B06-221102	3
Fagron	Furoato de mometasona	22C15-B06-223110	3
Fagron	Furoato de mometasona	22C15-B06-227594	1
Fagron	Furoato de mometasona	22C15-BO6-221102	1
Fagron	Furoato de mometasona	2517Q-07030	1
Fagron	Furoato de mometasona	2714U-07030	1
Fagron	Furoato de mometasona	2818A-07030	1
Fagron	Furoato de mometasona	3313A-07030	1
Fagron	Furoato de mometasona	334371	1
Fagron	Furoato de mometasona	335793	1
Fagron	Furoato de mometasona	339278	1
Fagron	Furoato de mometasona	347349	2
Fagron	Furoato de mometasona	352632	1
Fagron	Furoato de mometasona	354319	1
Fagron	Furoato de mometasona	4(18B19-B07-351001	1
Fagron	Furoato de mometasona	5(MOM001/0220)	1
Fagron	Furoato de mometasona	5/0715	1
Fagron	Furoato de mometasona	6071716	1
Fagron	Furoato de mometasona	701834-0001	1
Fagron	Furoato de mometasona	701834-0004	1
Fagron	Furoato de mometasona	83919-23-7	3
Fagron	Furoato de mometasona	B03-1968709	7
Fagron	Furoato de mometasona	B03-1970806	5
Fagron	Furoato de mometasona	B03-197086	2
Fagron	Furoato de mometasona	B05-2031001	2
Fagron	Furoato de mometasona	B05-2105403	1
Fagron	Furoato de mometasona	B12-1917600	1
Fagron	Furoato de mometasona	BO3-1968709	1
Fagron	Furoato de mometasona	Fagron21B26-B05-203101	1
Fagron	Furoato de mometasona	HM01620	1
Fagron	Furoato de mometasona	HMF010620	1
Fagron	Furoato de mometasona	HMF01620	2
Fagron	Furoato de mometasona	HMFO1620	1
Fagron	Furoato de mometasona	mom001/0220	1
Fagron	Furoato de mometasona	MOM001/0220	9
Fagron	Furoato de mometasona	MOM001/0317	4
Fagron	Furoato de mometasona	MOM003/0818	6
Fagron	Furoato de mometasona	MOM004/0716	4
Fagron	Furoato de mometasona	MOM004-0716	1
Fagron	Furoato de mometasona	MOM008/0915	3
Fagron	Furoato de mometasona	MOM010/0116	2
Fagron	Furoato de mometasona	MOM010/0118	8
Fagron	Furoato de mometasona	NS1513M	1
Fagron	Furoato de mometasona	NT1568M	3
Fagron	Furoato de mometasona	NU0698M	2
Fagron	Furoato de mometasona	NU2504M	1
Fargo / Gehe	Furoato de mometasona	20G24-B03	1
Fargon/AHD	Furoato de mometasona	18B19-B07-351001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fargon/AHD	Furoato de mometasona	18B19-B07-354319	1
Fargon/Gehe	Furoato de mometasona	20G24-B03-197086	2
Fargon	Furoato de mometasona	13H13-N04	1
Fargon	Furoato de mometasona	14h06-b07-298481	2
Fargon	Furoato de mometasona	16C24-B03-324852	1
Fargon	Furoato de mometasona	20G24-B03-196879	1
Fargron/Noweda	Furoato de mometasona	20G24-B03-197086	1
Finteler Apotheke	Furoato de mometasona	16028603	1
Finteler Apotheke	Furoato de mometasona	16028604	1
Fragon/Phoenix	Furoato de mometasona	19F13-B12-191762	1
Fragon/Sanacorp	Furoato de mometasona	16C24-B03-324851	1
Fragon/Sanacorp	Furoato de mometasona	17D19-B02-339277	2
Fragon/Sanacorp	Furoato de mometasona	17D19-B02-342642	1
Fragon/Sanacorp	Furoato de mometasona	17D19-B02-342643	2
Fragon/Sanacorp	Furoato de mometasona	17D19-B02-347348	1
Fragron/ Alliance	Furoato de mometasona	20G24-B03-196879	1
Gehe 07.12.18	Furoato de mometasona	1711027_02	1
GEHE 17.04.2014	Furoato de mometasona	13J23-N02	1
Gehe amax	Furoato de mometasona	17D19-B02-342643	1
Gehe amax	Furoato de mometasona	1906035-01	1
Gehe amax	Furoato de mometasona	19F13-B12-191761	1
Gehe/Caesar & Loretz GmbH	Furoato de mometasona	20003486021	1
Gehe/EuRoh	Furoato de mometasona	2003056-01	1
Gehe/europharm	Furoato de mometasona	2106014-01	6
Gehe	Furoato de mometasona	13D08-N06	1
Gehe	Furoato de mometasona	13H13-N04	2
Gehe	Furoato de mometasona	15B11-B03-304123	1
Gehe	Furoato de mometasona	15G08-B11-312233	1
Gehe	Furoato de mometasona	15G08-B11-317182	1
Gehe	Furoato de mometasona	16181704	1
Gehe	Furoato de mometasona	16353201	1
Gehe	Furoato de mometasona	16353206	1
Gehe	Furoato de mometasona	16353207	1
Gehe	Furoato de mometasona	16C24-B03-324852	1
Gehe	Furoato de mometasona	16C24-B03-327346	1
Gehe	Furoato de mometasona	16J24-B11-332112	2
Gehe	Furoato de mometasona	16J24-B11-335793	2
Gehe	Furoato de mometasona	17D19-B02	1
Gehe	Furoato de mometasona	17D19-B02-339278	1
Gehe	Furoato de mometasona	17D19-B02-342642	2
GEHE	Furoato de mometasona	17D19-B02-344776	1
GEHE	Furoato de mometasona	18026006	1
Gehe	Furoato de mometasona	18334101	1
gehe	Furoato de mometasona	18334104	1
Gehe	Furoato de mometasona	18B19-B07-352745	4
Gehe	Furoato de mometasona	18B19-B07-354318	1
Gehe	Furoato de mometasona	18B19-B07-354319	1
Gehe	Furoato de mometasona	18B19-B07-354319	1
Gehe	Furoato de mometasona	1906035-01	3
Gehe	Furoato de mometasona	19F13-B12-191761	1
Gehe	Furoato de mometasona	20003486002	1
Gehe	Furoato de mometasona	20003486026	1
Gehe	Furoato de mometasona	20003486034	1
gehe	Furoato de mometasona	20G24-Bo3-196879	1
Gehe	Furoato de mometasona	22C15-B06-221102	1
Geibo/ Fargron	Furoato de mometasona	16J24-b11-335792	1
Geibo	Furoato de mometasona	18B19-B07-354320	1
GUMO	Furoato de mometasona	2008002-01	5
Hedinger/Gehe	Furoato de mometasona	1896223	1
Holdermann	Furoato de mometasona	13D08-N06	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Holdermann	Furoato de mometasona	14C07-B05-29126	1
Ichthyol-Gesllschaft...	Furoato de mometasona	16J24-B11-335793	2
Jenne	Furoato de mometasona	18026012	1
Jenne	Furoato de mometasona	1802612	1
Jenne	Furoato de mometasona	20003486030	1
Jenne	Furoato de mometasona	20003486034	1
Jenne	Furoato de mometasona	21B26-805-203100	1
Kehr	Furoato de mometasona	16353206	1
Nachprüfung	Furoato de mometasona	1628604	1
Nachprüfung	Furoato de mometasona	16J24-B11-329817	1
Newchem / Gehe	Furoato de mometasona	16181715	1
Noveda	Furoato de mometasona	18334101	1
Noveda	Furoato de mometasona	20000787010	1
Noweda /Cealo	Furoato de mometasona	19200601	2
Noweda Taucha	Furoato de mometasona	20003486011	1
Noweda Taucha	Furoato de mometasona	2008002-01	2
Noweda	Furoato de mometasona	15G08-B11	1
Noweda	Furoato de mometasona	16C24-B03-328272	1
Noweda	Furoato de mometasona	16J24-B11-332111	1
Noweda	Furoato de mometasona	1711027-02	1
Noweda	Furoato de mometasona	17D19-B02-347349	1
Noweda	Furoato de mometasona	18026009	1
Noweda	Furoato de mometasona	18334110	1
Noweda	Furoato de mometasona	18B19-B07-351351	1
Noweda	Furoato de mometasona	20G24-B03-196879	1
Noweda	Furoato de mometasona	2106014-01	4
Noweda	Furoato de mometasona	21B26-B05-203100	2
Noweda	Furoato de mometasona	22C-B06	1
Noweda	Furoato de mometasona	23001247006	1
Phagron	Furoato de mometasona	19F13-B12-191761	1
Phoenix 03.08.2017	Furoato de mometasona	16C24-B03-328272	1
Phoenix	Furoato de mometasona	14C07-B05-291268	1
Phoenix	Furoato de mometasona	16181714	1
Phoenix	Furoato de mometasona	17D19-B02-339277	1
Phoenix	Furoato de mometasona	1810008-01	1
phoenix	Furoato de mometasona	18334108	1
Phoenix	Furoato de mometasona	18B19-B07-352745	1
Phoenix	Furoato de mometasona	19F13-B12-191760	1
Phoenix	Furoato de mometasona	20003486036	1
phoenix	Furoato de mometasona	2008002-01	1
Phoenix	Furoato de mometasona	20G24-B03-196879	1
Phoenix	Furoato de mometasona	3406	1
Phoenix	Furoato de mometasona	MOM004/0716	1
Phönix Gotha	Furoato de mometasona	1403015-01	1
Phönix	Furoato de mometasona	13/23-N02	2
Phönix	Furoato de mometasona	13D08-N06	1
Phönix	Furoato de mometasona	14E20-B04-291267	1
phönix	Furoato de mometasona	15B11-b03	1
Phönix	Furoato de mometasona	15G08-B11-322737	1
Phönix	Furoato de mometasona	16C24-B03	1
Phönix	Furoato de mometasona	16c24-b03-327346	1
Phönix	Furoato de mometasona	171102702	1
Phönix	Furoato de mometasona	17D19-B02-342642	1
Phönix	Furoato de mometasona	18026012	1
Phönix	Furoato de mometasona	1906035-01	2
Phönix	Furoato de mometasona	20003486017	1
Phönix	Furoato de mometasona	20003486018	1
Phönix	Furoato de mometasona	2008002-01	4
Phönix	Furoato de mometasona	20G24-B03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
phönix	Furoato de mometasona	2106014-01	1
Phönix	Furoato de mometasona	2106014-01	1
Phönx	Furoato de mometasona	2008002-01	3
Sana	Furoato de mometasona	MF-18009(JM-01)001	1
Sanacorp /Fargron	Furoato de mometasona	15G08-B11-310864	1
Sanacorp /Fargron	Furoato de mometasona	16J24-B11-335792	1
Sanacorp	Furoato de mometasona	1/AKD4	1
Sanacorp	Furoato de mometasona	14E20-B04-291267	1
Sanacorp	Furoato de mometasona	15189801	1
Sanacorp	Furoato de mometasona	16353211	1
Sanacorp	Furoato de mometasona	17D19-B02-339276	1
Sanacorp	Furoato de mometasona	17D19-B02-344776	2
Sanacorp	Furoato de mometasona	18026001	1
Sanacorp	Furoato de mometasona	18B19-B07-354319	2
Sanacorp	Furoato de mometasona	20000787007	1
Sanacorp	Furoato de mometasona	20G24-B03-197086	2
Sanacorp	Furoato de mometasona	21B26-B05	1
Sanacorp	Furoato de mometasona	21B26-B05-203100	2
Sanacorp	Furoato de mometasona	22C15-B06-227594	1
Sanacorp	Furoato de mometasona	23001247006	1
Sanacorp	Furoato de mometasona	23F15-B02-234650	1
Sanacorp	Furoato de mometasona	MOM001/0317	1
SanacorpWE:12.01.201…	Furoato de mometasona	16028602	1
sidonia	Furoato de mometasona	18334110	1
Symbiotic/Phoenix	Furoato de mometasona	2001040-01	2
Symbiotica / Gehe	Furoato de mometasona	MOM008/0915	2
Symbiotica Malaysia/ AHD	Furoato de mometasona	2001040-01	1
Symbiotica/Phoenix	Furoato de mometasona	MOM001/0317	1
Symbiotica/Phoenix	Furoato de mometasona	MOM003/0818	2

- 233 334 spectra from 1514 *Apo-Ident* customers from a total of 48 750 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Furoato de mometasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Furoato de mometasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	545	0	152 417
Type B	0	903	1	201 180
Type C	0	2724	9	233 334

The substance/substance group *Furoato de mometasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8991 %)
Type B	100.0000 % (> 99.9912 %)	99.8894 % (> 99.5575 %)
Type C	100.0000 % (> 99.9007 %)	99.6707 % (> 99.5609 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20850	22433	5,72	180,74
21602	22433	9,36	181,96
22238	22238	0,00	179,21
22433	22433	0,00	183,20
22887	23136	8,35	182,86
23046	23046	0,00	178,85
23136	23136	0,00	182,43
26766	26766	0,00	183,34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Furosemida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20944-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Furosemida; Furosemidum

Special notes

When selecting the *Furosemida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Furosemida	6	3	29

Second-stage model

For differentiation of the substance/substance group *Furosemida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Furosemida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	157,47	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Furosemida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Furosemida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Furosemida	13A22-N08	20944	40	1401379
Fagron	Furosemida	14K10-B02-301746	21819	60	20141215
Fagron	Furosemida	17D06-B01-338982	23940	40	20170626
Fagron	Furosemida	19I27-F04-366906	25044	40	20191218
Fagron	Furosemida	22L05-B06-225369	26607	40	20230104
Fagron	Furosemida	22L05-B06-225369	26607SI	20	20230104
Fagron	Furosemida	23G05-B14-230372	26977	40	20230830

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Furosemida*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Furosemida*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Furosemida	16B15-B06-322860	23083	40
Fagron	Furosemida	20G10-F10-373076	25442	40
Fagron	Furosemida	21K30-B02-221074	26168	40
Fagron	Furosemida	16B15-B06-322860	23084	40
Fagron	Furosemida	21K30-B02-221074	26168SI	20
Fagron	Furosemida	23G05-B14-230372	26977SI†	20

- 201 884 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 74 spectra from 56 *Apo-Ident* customers from 35 batches from the substance/substance group *Furosemida*.
- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Furosemida	20G10-F10-373076	1
	Furosemida	20G10-F10-374131	2
	Furosemida	-23201008	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Furosemida	23G05-B14230372	1
	Furosemida	23G05-B14-230372	1
AHC	Furosemida	23G05-B14-230372	1
Alliance Healthcare/…	Furosemida	12/13-N06	1
Caelo	Furosemida	16B15-B06	1
Caelo	Furosemida	20G10-F10-374131	1
Fagron	Furosemida	1095H2RI	1
Fagron	Furosemida	11K21-N26	1
Fagron	Furosemida	12A18-N03	1
Fagron	Furosemida	12I13-No6	1
Fagron	Furosemida	13A22-N08	4
Fagron	Furosemida	13E28-B40	2
Fagron	Furosemida	13E28-B40-289433	1
Fagron	Furosemida	13E28-B40-295538	1
Fagron	Furosemida	14K10-B02-301746	1
Fagron	Furosemida	15L10B02316506	1
Fagron	Furosemida	15L10-B02-316506	2
Fagron	Furosemida	16/26-B04-329253	2
Fagron	Furosemida	17d06-b01-335672	1
Fagron	Furosemida	17D06-B01-335672	2
Fagron	Furosemida	17D06-B01-338982	1
Fagron	Furosemida	18C27-B02	1
Fagron	Furosemida	18C27-B02-348148	2
Fagron	Furosemida	19I27-F04-366906	2
Fagron	Furosemida	-20200004	1
Fagron	Furosemida	20G10-F10	5
Fagron	Furosemida	20G10-F10-3730706	2
Fagron	Furosemida	20G10-F10373076	1
Fagron	Furosemida	20G10-F10-373076	16
Fagron	Furosemida	20G10-F10-373079	1
Fagron	Furosemida	20G10-F10-374131	3
Fagron	Furosemida	AM20216066	1
Fagron	Furosemida	F10-3730706	1
Fagron	Furosemida	FRD-2B-202004	2
Fagron	Furosemida	FUR-1A-192016	1
IPCA/Noweda	Furosemida	11D29-N08	1
Phoenix	Furosemida	17D06-B01-338982	1
Sanacorp	Furosemida	FUR-1A-192016	1

- 235 993 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Furosemida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Furosemida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	200	0	201 884
Type C	0	74	0	235 993

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Furosemida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.8919 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20944	20944	0,00	375,75
21819	20944	11,31	372,08
23940	20944	10,08	374,24
25044	20944	4,36	380,19
26607	20944	7,97	383,26
26977	20944	8,51	385,65

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gabapentina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005490-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gabapentina; Gabapentinum

Special notes

When selecting the *Gabapentina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gabapentina	3	2	4

Second-stage model

For differentiation of the substance/substance group *Gabapentina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gabapentina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ácido tranexâmico	76,20	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gabapentina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gabapentina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Gabapentina	21G13-B17-215252	26079	40	20220329
Hikal Ltd.	Gabapentina	G71010620/077	25833	50	2203054
Hikal Ltd.	Gabapentina	B71010621/105	25898	50	20211111

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 3 reference samples from the substance/substance group *Gabapentina*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 822 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 7 reference samples from the substance/substance group *Gabapentina*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Gabapentina	22H02-B04-228420	26614	40
MEDICHEM S.A.	Gabapentina	A-180101	25837	50
Fagron	Gabapentina	21G13-B17-215252	26079SI†	40
Fagron	Gabapentina	22H02-B04-228420	26614SI	20
Hikal Ltd.	Gabapentina	G71010620/077	25833SI†	10
Hikal Ltd.	Gabapentina	B71010621/105	25898SI†	10
MEDICHEM S.A.	Gabapentina	A-180101	25837SI	10

- 201 904 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Gabapentina*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gabapentina	22H02-B04-228420	3
	Gabapentina	B04-2284200	4
Fagron	Gabapentina	21G13-B17-2152502	1
INRESA/INRESA	Gabapentina	B71010621/409	1

- 236 058 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gabapentina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gabapentina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	180	0	201 904
Type C	0	9	0	236 058

The substance/substance group *Gabapentina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25833	25833	0,00	144,97
25898	25833	15,75	152,28
26079	25833	16,84	151,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Galactose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20326-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Galactose; Galactosum

Special notes

When selecting the *Galactose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Galactose	4	3	27

Second-stage model

For differentiation of the substance/substance group *Galactose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Galactose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	68,41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Galactose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Galactose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Galactose	13I13-B40-287993	21762	60	AR-15-FG-008936-01
Fagron	Galactose	14H05-B09-310972	22259	60	20140818
Fagron	Galactose	18F14-B02-355816	25179	40	20181212
Fagron	Galactose	23H08-F01-385354	27032	40	20231009
Fagron	Galactose	23H08-F01-385354	27032SI	20	20231009

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Galactose*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 742 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Galactose*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Galactose	15G13-B04-320810	23106	40
Fagron	Galactose	19G12-F50-373175	25443	40
Fagron	Galactose	24H01-B08-001699	27422	40
Fagron	Galactose	15G13-B04-320810	23595	40
Fagron	Galactose	24H01-B08-001699	27422SI	20

- 201 904 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 39 spectra from 5 *Apo-Ident* customers from 28 batches from the substance/substance group *Galactose*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Applichem	Galactose	2L009814	1
Fagron	Galactose	16G22-B01-329906	1
Falcento	Galactose	10440003	1
Falcento	Galactose	12223PF4	2
Falcento	Galactose	1223PF4	3
Falcento	Galactose	122PF4	1
Falcento	Galactose	13223PF4	1
Falcento	Galactose	2014	1
Falcento	Galactose	2223PF4	3
Falcento	Galactose	222PF4	1
Falcento	Galactose	233619PF5	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
falcento	Galactose	322619PF5	1
Falcento	Galactose	48223PF2	1
Falcento	Galactose	5223PF4	3
Falcento	Galactose	72619PF7	1
Falcento	Galactose	82619PF64743/16	1
Falcento	Galactose	82619PF7	1
Falcento	Galactose	92619PF64744/16	1
inalco	Galactose	212619PF5	1
inalco	Galactose	32619PF8	1
inalco	Galactose	42619PF4	1
Phönix 04.03.2014	Galactose		1
Phönix	Galactose	39223PF3	1
Unisan	Galactose	382619PF5	1
Unisan	Galactose	432619PF5	1
Unisan	Galactose	442619PF5	1
vwr chemicals	Galactose	1F012304	1
VWR	Galactose	9Y013597	5

- 236 028 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Galactose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Galactose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	180	0	201 904
Type C	0	39	0	236 028

The substance/substance group *Galactose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.6154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21762	21762	0,00	190,13
22259	21762	18,46	178,48
25179	21762	15,17	186,12
27032	21762	19,20	190,07

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Galato de bismuto, básico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21252-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Galato de bismuto, básico; Bismuthi subgallas

Special notes

When selecting the *Galato de bismuto, básico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Galato de bismuto, básico	6	5	247

Second-stage model

For differentiation of the substance/substance group *Galato de bismuto, básico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Galato de bismuto, básico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	79,94	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Galato de bismuto, básico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Galato de bismuto, básico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Galato de bismuto, básico	13179105	21252	40	1412254
Caelo	Galato de bismuto, básico	13179105	21553	60	20130701
Caelo	Galato de bismuto, básico	170041	23359	40	20170214*
Caelo	Galato de bismuto, básico	17004102	23372	40	20170214
Caelo	Galato de bismuto, básico	20000903	25204	40	20200331*
Fagron	Galato de bismuto, básico	15B02-B04-309481	22597	40	20150226
Fagron	Galato de bismuto, básico	15J26-B02-317883	22598	40	20151102

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Galato de bismuto, básico*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 662 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 230 spectra of 6 reference samples from the substance/substance group *Galato de bismuto, básico*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Galato de bismuto, básico	191063	24714	40
Caelo	Galato de bismuto, básico	21003110	25845	50
Fagron	Galato de bismuto, básico	16K17-B04-335597	23570	40
Fagron	Galato de bismuto, básico	19K28-B02-196432	25186	40
Fagron	Galato de bismuto, básico	22I21-B04-223756	26617	40
Fagron	Galato de bismuto, básico	22I21-B04-223756	26617SI	20

- 201 854 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 880 spectra from 445 *Apo-Ident* customers from 264 batches from the substance/substance group *Galato de bismuto, básico*.

- Among them are spectra of independent samples from 247 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Galato de bismuto, básico	2022003849	2
	Galato de bismuto, básico	2023001183	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Galato de bismuto, básico	202300183	1
	Galato de bismuto, básico	2023004222	1
	Galato de bismuto, básico	21003110005	1
	Galato de bismuto, básico	21003110009	1
	Galato de bismuto, básico	21003110010	2
	Galato de bismuto, básico	21003110013	1
	Galato de bismuto, básico	21003110015	1
	Galato de bismuto, básico	21003110017	1
	Galato de bismuto, básico	21G21-B03-213570	2
	Galato de bismuto, básico	22I21-B04-228625	1
	Galato de bismuto, básico	22121-B04-228625	1
	Galato de bismuto, básico	B04-2286205	3
5N Plus GmbH / Ebert	Galato de bismuto, básico	18040801	1
5N Plus GmbH/Phoenix	Galato de bismuto, básico	2020000872	1
ahd/lamotte	Galato de bismuto, básico	13718_b13_292058	1
Alliance H.	Galato de bismuto, básico	15080602	1
Alliance Healthcare	Galato de bismuto, básico	13D19-N02	2
Alliance	Galato de bismuto, básico	12172402	1
Allianz Healthcare	Galato de bismuto, básico	15200911	1
Allianz Healthcare	Galato de bismuto, básico	17259517	1
Anzag	Galato de bismuto, básico	2012000059	2
apomix	Galato de bismuto, básico	13D19-N02	1
Bombastus	Galato de bismuto, básico	13/18-B13-292058	1
Bombastus	Galato de bismuto, básico	13G10-N12	1
Caelo	Galato de bismuto, básico		1
Caelo	Galato de bismuto, básico	10135109	1
Caelo	Galato de bismuto, básico	10D23-N05	1
Caelo	Galato de bismuto, básico	11127101	1
Caelo	Galato de bismuto, básico	11127104	1
Caelo	Galato de bismuto, básico	1127203	1
Caelo	Galato de bismuto, básico	12166901	2
Caelo	Galato de bismuto, básico	1217240	1
Caelo	Galato de bismuto, básico	12172401	1
Caelo	Galato de bismuto, básico	12172402	4
Caelo	Galato de bismuto, básico	12172409	6
Caelo	Galato de bismuto, básico	12172412	5
Caelo	Galato de bismuto, básico	12c13-n03	1
Caelo	Galato de bismuto, básico	12C13-N03	1
Caelo	Galato de bismuto, básico	12c13-no3	1
Caelo	Galato de bismuto, básico	12E16-N03	1
Caelo	Galato de bismuto, básico	12I13-N11	1
Caelo	Galato de bismuto, básico	13/18-B13-292057	1
Caelo	Galato de bismuto, básico	13/18-B13-292058	1
Caelo	Galato de bismuto, básico	13179101	2
Caelo	Galato de bismuto, básico	13179105	1
Caelo	Galato de bismuto, básico	13179111	6
Caelo	Galato de bismuto, básico	13D19-N02	2
Caelo	Galato de bismuto, básico	13I18-B13	1
Caelo	Galato de bismuto, básico	13I18-B13-294108	2
Caelo	Galato de bismuto, básico	14224103	4
Caelo	Galato de bismuto, básico	14224105	2
Caelo	Galato de bismuto, básico	15080602	3
Caelo	Galato de bismuto, básico	15080603	1
Caelo	Galato de bismuto, básico	15080606	10
Caelo	Galato de bismuto, básico	15200904	3
Caelo	Galato de bismuto, básico	15200905	1
Caelo	Galato de bismuto, básico	15200907	1
Caelo	Galato de bismuto, básico	15200910	2
Caelo	Galato de bismuto, básico	15200911	7
Caelo	Galato de bismuto, básico	15200913	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Galato de bismuto, básico	1520910	1
Caelo	Galato de bismuto, básico	1520913	1
Caelo	Galato de bismuto, básico	15B02-B04-304408	1
Caelo	Galato de bismuto, básico	15B02B04304413	1
Caelo	Galato de bismuto, básico	15B02-B04-309481	2
Caelo	Galato de bismuto, básico	15J26_B02-321313	1
Caelo	Galato de bismuto, básico	15J26-B02-320473	1
Caelo	Galato de bismuto, básico	15J26-B02-320479	1
Caelo	Galato de bismuto, básico	1603810	1
Caelo	Galato de bismuto, básico	16038308	7
Caelo	Galato de bismuto, básico	16038310	7
Caelo	Galato de bismuto, básico	16038312	9
Caelo	Galato de bismuto, básico	16K17-B04-335597	1
Caelo	Galato de bismuto, básico	17/26-B01-340556	1
Caelo	Galato de bismuto, básico	17004102	10
Caelo	Galato de bismuto, básico	17004106	10
Caelo	Galato de bismuto, básico	17004107	5
Caelo	Galato de bismuto, básico	17004109	9
Caelo	Galato de bismuto, básico	17004112	11
Caelo	Galato de bismuto, básico	1725909	1
Caelo	Galato de bismuto, básico	17259503	2
Caelo	Galato de bismuto, básico	17259505	4
Caelo	Galato de bismuto, básico	17259509	6
Caelo	Galato de bismuto, básico	17259510	6
Caelo	Galato de bismuto, básico	17259513	5
Caelo	Galato de bismuto, básico	17259517	7
Caelo	Galato de bismuto, básico	17259519	3
Caelo	Galato de bismuto, básico	17E16-B02-336992	1
Caelo	Galato de bismuto, básico	17-E16-B02-336992	1
Caelo	Galato de bismuto, básico	17I26-B01-341866	1
Caelo	Galato de bismuto, básico	18040801	11
Caelo	Galato de bismuto, básico	18A29-B06	1
Caelo	Galato de bismuto, básico	18A29-B06-346305	2
Caelo	Galato de bismuto, básico	18A29-B346305	1
Caelo	Galato de bismuto, básico	191063002	21
Caelo	Galato de bismuto, básico	191063004	6
Caelo	Galato de bismuto, básico	191063005	1
Caelo	Galato de bismuto, básico	191063006	8
Caelo	Galato de bismuto, básico	19106301	8
Caelo	Galato de bismuto, básico	19106302	6
Caelo	Galato de bismuto, básico	19B05-B09-191019	1
Caelo	Galato de bismuto, básico	20004232001	4
Caelo	Galato de bismuto, básico	20004232002	2
Caelo	Galato de bismuto, básico	20004232004	3
Caelo	Galato de bismuto, básico	2004232006	1
Caelo	Galato de bismuto, básico	2012006724	1
Caelo	Galato de bismuto, básico	2017002570	1
Caelo	Galato de bismuto, básico	21000126001	5
Caelo	Galato de bismuto, básico	21003110002	7
Caelo	Galato de bismuto, básico	21003110005	3
Caelo	Galato de bismuto, básico	21003110006	6
Caelo	Galato de bismuto, básico	21003110009	2
Caelo	Galato de bismuto, básico	21003110010	2
Caelo	Galato de bismuto, básico	21003110013	1
Caelo	Galato de bismuto, básico	220511(21000126001)	1
Caelo	Galato de bismuto, básico	23121410	1
Caelo	Galato de bismuto, básico	2414E-01185	1
Caelo	Galato de bismuto, básico	26011903	1
Caelo	Galato de bismuto, básico	5208I-01185	1
Caelo	Galato de bismuto, básico	62183516	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Galato de bismuto, básico	81297468	5
Caelo	Galato de bismuto, básico	8129768	1
Caelo	Galato de bismuto, básico	9205701	1
Caelo	Galato de bismuto, básico	9205703	2
Caelo	Galato de bismuto, básico	92057409	1
Caelo	Galato de bismuto, básico	9K26-N10	2
Caelo	Galato de bismuto, básico	B02-1964302	2
Caelo	Galato de bismuto, básico	B-150513-1	1
Caesar & Loretz GmbH...	Galato de bismuto, básico	17259505	1
Caesar & Loretz GmbH/Gehe	Galato de bismuto, básico	17259509	1
Caesar & Loretz GmbH/Gehe	Galato de bismuto, básico	191063006	1
Caesar & Loretz GmbH/Gehe	Galato de bismuto, básico	19106301	1
Caesar & Loretz GmbH/Gehe	Galato de bismuto, básico	21000126001	2
Caesar & Loretz GmbH...	Galato de bismuto, básico	20004232004	1
Caesar & Loretz GmbH...	Galato de bismuto, básico	191063004	2
Caesar & Loretz GmbH...	Galato de bismuto, básico	191063006	1
Caesar & Loretz GmbH	Galato de bismuto, básico	16038312	2
Caesar & Loretz GmbH	Galato de bismuto, básico	17004102	1
Caesar & Loretz GmbH	Galato de bismuto, básico	17259509	2
Caesar & Loretz GmbH	Galato de bismuto, básico	17259510	2
Caesar & Loretz GmbH	Galato de bismuto, básico	17259513	3
Caesar & Loretz GmbH	Galato de bismuto, básico	191063002	4
Caesar & Loretz GmbH	Galato de bismuto, básico	191063004	2
Caesar & Loretz GmbH	Galato de bismuto, básico	191063006	6
Caesar & Loretz GmbH	Galato de bismuto, básico	19106301	3
Caesar & Loretz GmbH	Galato de bismuto, básico	20004232001	3
Caesar & Loretz GmbH	Galato de bismuto, básico	20004232004	2
Caesar & Loretz GmbH	Galato de bismuto, básico	21000126001	5
Caesar & Loretz GmbH	Galato de bismuto, básico	21003110002	5
Caesar & Loretz GmbH	Galato de bismuto, básico	21003110006	8
Caesar & Loretz GmbH	Galato de bismuto, básico	21003110009	1
Caesar/Ebert	Galato de bismuto, básico	17259509	1
Euro OTC	Galato de bismuto, básico	16K17-B04-335597	3
Fagro/Gehe	Galato de bismuto, básico	2018005145	1
Fagron	Galato de bismuto, básico		3
Fagron	Galato de bismuto, básico	10H31-N01	1
Fagron	Galato de bismuto, básico	114101-0003	1
Fagron	Galato de bismuto, básico	11F15-N03	1
Fagron	Galato de bismuto, básico	12/13-N11	1
Fagron	Galato de bismuto, básico	12B02-B04-304408	1
Fagron	Galato de bismuto, básico	12C13-N03	4
Fagron	Galato de bismuto, básico	12E16-NO3	1
Fagron	Galato de bismuto, básico	12K26-N01	3
Fagron	Galato de bismuto, básico	13/18-B13-292057	2
Fagron	Galato de bismuto, básico	13/18-B-13-292057	1
Fagron	Galato de bismuto, básico	13/18-B13-292058	3
Fagron	Galato de bismuto, básico	13/18-B13294098	1
Fagron	Galato de bismuto, básico	13/18-B13-294098	2
Fagron	Galato de bismuto, básico	13/18-B13-294108	3
Fagron	Galato de bismuto, básico	13179111	1
Fagron	Galato de bismuto, básico	1318-B13-292057	2
Fagron	Galato de bismuto, básico	1318b13292058	1
Fagron	Galato de bismuto, básico	1318B1329409	1
Fagron	Galato de bismuto, básico	1318B13294108	1
Fagron	Galato de bismuto, básico	13D19-N02	3
Fagron	Galato de bismuto, básico	13E21-N03	2
Fagron	Galato de bismuto, básico	13F10-N12	1
Fagron	Galato de bismuto, básico	13G10-N12	4
Fagron	Galato de bismuto, básico	13I18-B13	5
Fagron	Galato de bismuto, básico	13I18-b13-292057	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Galato de bismuto, básico	13I18-B13-292057	2
Fagron	Galato de bismuto, básico	13I18-B13-292058	1
Fagron	Galato de bismuto, básico	13I18-B13-294098	4
Fagron	Galato de bismuto, básico	13i18-b13-294108	1
Fagron	Galato de bismuto, básico	13I18-B13-294108	6
Fagron	Galato de bismuto, básico	13K08-N03	4
Fagron	Galato de bismuto, básico	14H13-B07	1
Fagron	Galato de bismuto, básico	14H13B07303639	1
Fagron	Galato de bismuto, básico	14H13-B07-303639	6
Fagron	Galato de bismuto, básico	15/26-B02-320473	1
Fagron	Galato de bismuto, básico	15/26-B02-321313	1
Fagron	Galato de bismuto, básico	15126-B02-321313	1
Fagron	Galato de bismuto, básico	15B02-B04	3
Fagron	Galato de bismuto, básico	15B02-B04-209481	1
Fagron	Galato de bismuto, básico	15b02b04304408	1
Fagron	Galato de bismuto, básico	15B02-B04-304408	9
Fagron	Galato de bismuto, básico	15B02-B04-304413	5
Fagron	Galato de bismuto, básico	15b02-B04-309481	1
Fagron	Galato de bismuto, básico	15B02B04309481	1
Fagron	Galato de bismuto, básico	15B02-B04-309481	4
Fagron	Galato de bismuto, básico	15B02-B04-311878	1
Fagron	Galato de bismuto, básico	15C27-B02-311879	1
Fagron	Galato de bismuto, básico	15H05-B07	1
Fagron	Galato de bismuto, básico	15H05-B07-311880	5
Fagron	Galato de bismuto, básico	15I26-B02-325472	1
Fagron	Galato de bismuto, básico	15J26-B02	5
Fagron	Galato de bismuto, básico	15J26-B022	1
Fagron	Galato de bismuto, básico	15J26-B02-317883	9
Fagron	Galato de bismuto, básico	15J26-B02-320473	5
Fagron	Galato de bismuto, básico	15j26-b02-321313	1
Fagron	Galato de bismuto, básico	15J26-B02-321313	6
Fagron	Galato de bismuto, básico	15J26-B02-325450	1
Fagron	Galato de bismuto, básico	15J26-B02-325472	9
Fagron	Galato de bismuto, básico	15J26-BO2-321313	2
Fagron	Galato de bismuto, básico	16K17B04	1
Fagron	Galato de bismuto, básico	16K17-B04	1
Fagron	Galato de bismuto, básico	16K17-B04-3355593	1
Fagron	Galato de bismuto, básico	16K17B04335597	2
Fagron	Galato de bismuto, básico	16K17-B04-335597	11
Fagron	Galato de bismuto, básico	17/26-B01-340556	4
Fagron	Galato de bismuto, básico	17/26-B01-341866	1
Fagron	Galato de bismuto, básico	1726B01341866	1
Fagron	Galato de bismuto, básico	17E16-B02	4
Fagron	Galato de bismuto, básico	17E16-B02-336968	1
Fagron	Galato de bismuto, básico	17E16-B02-336992	3
Fagron	Galato de bismuto, básico	17G06-B10-355772	1
Fagron	Galato de bismuto, básico	17i26-B01	1
Fagron	Galato de bismuto, básico	17I26-B01-340552	4
Fagron	Galato de bismuto, básico	17I26-B01-340556	6
Fagron	Galato de bismuto, básico	17I26-B01-341866	5
Fagron	Galato de bismuto, básico	180307BB/2016006984	1
Fagron	Galato de bismuto, básico	180808186	1
Fagron	Galato de bismuto, básico	18A29-B06	2
Fagron	Galato de bismuto, básico	18A29-B06-3460303	1
Fagron	Galato de bismuto, básico	18A29-B06-346303	1
Fagron	Galato de bismuto, básico	18A29B06-346305	1
Fagron	Galato de bismuto, básico	18A29-B06-346305	8
Fagron	Galato de bismuto, básico	18A29-BO6-346305	1
Fagron	Galato de bismuto, básico	18G06-B10	2
Fagron	Galato de bismuto, básico	18G06-B10-352463	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Galato de bismuto, básico	18G06-B10-352486	3
Fagron	Galato de bismuto, básico	18G06-B10-353902	2
Fagron	Galato de bismuto, básico	18G06-B10-353916	6
Fagron	Galato de bismuto, básico	18G06B10355772	2
Fagron	Galato de bismuto, básico	18G06-B10-355772	6
Fagron	Galato de bismuto, básico	18K29-B06-346303	1
Fagron	Galato de bismuto, básico	191022	1
Fagron	Galato de bismuto, básico	19B05-B09-191019	4
Fagron	Galato de bismuto, básico	19B05-B09-191022	8
Fagron	Galato de bismuto, básico	19k28-B02	1
Fagron	Galato de bismuto, básico	19K28-B02	4
Fagron	Galato de bismuto, básico	19K28-B02-196431	12
Fagron	Galato de bismuto, básico	19k28b02196432	1
Fagron	Galato de bismuto, básico	19K28-B02-196432	18
Fagron	Galato de bismuto, básico	19k28-B02-201353	1
Fagron	Galato de bismuto, básico	19K28-B02-201353	2
Fagron	Galato de bismuto, básico	19K28Bo2-196432	1
Fagron	Galato de bismuto, básico	2010002685	2
Fagron	Galato de bismuto, básico	20114b10202382	1
Fagron	Galato de bismuto, básico	2012000059	3
Fagron	Galato de bismuto, básico	2012006724	2
Fagron	Galato de bismuto, básico	2013006220	1
Fagron	Galato de bismuto, básico	2014006082	1
Fagron	Galato de bismuto, básico	2015000361	3
Fagron	Galato de bismuto, básico	2015000866	1
Fagron	Galato de bismuto, básico	2015007568	4
Fagron	Galato de bismuto, básico	2016006984	1
Fagron	Galato de bismuto, básico	2017002570	1
Fagron	Galato de bismuto, básico	2017006945	4
Fagron	Galato de bismuto, básico	2018000237	2
Fagron	Galato de bismuto, básico	2018005145	7
Fagron	Galato de bismuto, básico	2019001542	11
Fagron	Galato de bismuto, básico	2020004951	2
Fagron	Galato de bismuto, básico	2021001320	1
Fagron	Galato de bismuto, básico	20I14_B10-202382	1
Fagron	Galato de bismuto, básico	20I14-B10	1
Fagron	Galato de bismuto, básico	20i14-B10-2023802	1
Fagron	Galato de bismuto, básico	20I14-B10-202382	4
Fagron	Galato de bismuto, básico	21F11-B99	2
Fagron	Galato de bismuto, básico	21F11-B99-215303	1
Fagron	Galato de bismuto, básico	21f11-b99-215304	1
Fagron	Galato de bismuto, básico	21F11-B99-215304	5
Fagron	Galato de bismuto, básico	21G21-B03	2
Fagron	Galato de bismuto, básico	21g21b0321213570	1
Fagron	Galato de bismuto, básico	21G21-B03-213244	1
Fagron	Galato de bismuto, básico	21G21-B03-213570	8
Fagron	Galato de bismuto, básico	21G21-B03-215370	1
Fagron	Galato de bismuto, básico	22121-B04-223756	1
Fagron	Galato de bismuto, básico	22I21-B04-223683	1
Fagron	Galato de bismuto, básico	22I21-B04-223756	2
Fagron	Galato de bismuto, básico	22121-B04-223756	1
Fagron	Galato de bismuto, básico	26-B01-340552	1
Fagron	Galato de bismuto, básico	325472	1
Fagron	Galato de bismuto, básico	411092-3-P	1
Fagron	Galato de bismuto, básico	5121	1
Fagron	Galato de bismuto, básico	B02-1964302	1
Fagron	Galato de bismuto, básico	B02-2013503	1
Fagron	Galato de bismuto, básico	B02-201353	1
Fagron	Galato de bismuto, básico	b03-2135700	1
Fagron	Galato de bismuto, básico	B09-1910109	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Galato de bismuto, básico	B10-2023802	1
Fagron	Galato de bismuto, básico	BO2-1964302	1
Fagron	Galato de bismuto, básico	BO3-2135700	1
Fargon GmbH & Co.KG	Galato de bismuto, básico	15J26-B02-321313	2
Fargon/ Noweda	Galato de bismuto, básico	15B02-B04-309481	1
Fargon/ Sanacorp	Galato de bismuto, básico	19K28-BO2-196432	1
Fargon/Sanacorp	Galato de bismuto, básico	18A29-B06-346305	1
Fargon	Galato de bismuto, básico	13/18-B13-294108	1
Fargron	Galato de bismuto, básico	13D19-N02	1
Fargron	Galato de bismuto, básico	16k17-b04-335597	1
Frago/Noweda	Galato de bismuto, básico	16K17-B04-335597	1
Fragon/Sanacorp	Galato de bismuto, básico	16K17-B04-335593	1
Fragon/Sanacorp	Galato de bismuto, básico	17/26-B01-340552	1
Fragon/Sanacorp	Galato de bismuto, básico	18A-29-B06-346303	1
Fragon	Galato de bismuto, básico	19B05-B09-191022	1
Fragon	Galato de bismuto, básico	19K28-B02-19643	1
Fragon	Galato de bismuto, básico	19K28-B02-1964301	1
Fragon	Galato de bismuto, básico	19K28-B02-196431	2
Fragon	Galato de bismuto, básico	19K28-B02-196432	1
Gehe amax	Galato de bismuto, básico	15J26-B02-325450	1
Gehe	Galato de bismuto, básico	12172401	1
Gehe	Galato de bismuto, básico	15080607	1
Gehe	Galato de bismuto, básico	15J26-B02-317883	1
GEHE	Galato de bismuto, básico	17259509	1
Gehe	Galato de bismuto, básico	17E16-B02-336992	1
GEHE	Galato de bismuto, básico	18040801	1
GEHE	Galato de bismuto, básico	18A29-B06	2
Gehe	Galato de bismuto, básico	2015007568	1
Hedinger	Galato de bismuto, básico	16038310	1
Infectopharm	Galato de bismuto, básico	14224103	1
Kehr	Galato de bismuto, básico	17I26-B01-341866	1
Klenk	Galato de bismuto, básico	12E16-N03	1
L12	Galato de bismuto, básico	16038308	1
Martinus Apotheke	Galato de bismuto, básico	keine	1
Noweda	Galato de bismuto, básico	17/26-B01-341866	1
Noweda	Galato de bismuto, básico	18A29-B06-346303	1
Noweda	Galato de bismuto, básico	19K28-B02-196431	1
Noweda	Galato de bismuto, básico	19K28-B02-196432	1
Noweda	Galato de bismuto, básico	19K28-B02-201353	1
Noweda	Galato de bismuto, básico	20004232001	1
Noweda	Galato de bismuto, básico	21003110010	1
PHOENIX am 17.01.2014	Galato de bismuto, básico	2012006724	1
Phoenix, Jembke	Galato de bismuto, básico	10135101	1
Phoenix	Galato de bismuto, básico	1520913	1
Phoenix	Galato de bismuto, básico	191063002	1
Phönix	Galato de bismuto, básico	12-13-N11	1
Phönix	Galato de bismuto, básico	12E16-N03	1
phönix	Galato de bismuto, básico	15J26-B02-325450	1
Phönix	Galato de bismuto, básico	17259505	2
Phönix	Galato de bismuto, básico	19K28-B02	1
Phönix	Galato de bismuto, básico	19K28-B02-196432	1
Phönix	Galato de bismuto, básico	21g21-b03-213570	1
Sanacorp 03.01.22 23,00EUR	Galato de bismuto, básico	220103BE	1
Sanacorp 28.06.2017 ...	Galato de bismuto, básico	2015007568	1
Sanacorp	Galato de bismuto, básico	12/13-N11	1
sanacorp	Galato de bismuto, básico	13/1818B13-292057	1
Sanacorp	Galato de bismuto, básico	13D19-N02	1
Sanacorp	Galato de bismuto, básico	18A29-B06-346305	1
Sanacorp	Galato de bismuto, básico	19K28-B02-2013503	1
Sanacorp	Galato de bismuto, básico	2018005145	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Galato de bismuto, básico	2019001542-B02-201353	1
Sanacorp	Galato de bismuto, básico	B02-2013503	1
Sidonia	Galato de bismuto, básico	15200904	1
Sidonia	Galato de bismuto, básico	15J-26-B02-325450	1
Sidonia	Galato de bismuto, básico	17004107	3
siehe WE-Prüfprotokoll	Galato de bismuto, básico	4/09	1

- 235 187 spectra from 1515 *Apo-Ident* customers from a total of 48 995 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Galato de bismuto, básico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Galato de bismuto, básico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	230	0	201 854
Type C	0	877	3	235 187

The substance/substance group *Galato de bismuto, básico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.3913 %)
Type C	100.0000 % (> 99.9007 %)	99.6591 % (> 99.3182 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21252	21252	0,00	71,55
21553	21252	5,91	70,37
22597	25204	10,31	68,73
22598	25204	9,59	69,22
23359	23359	0,00	70,71
23372	21252	9,39	68,13
25204	25204	0,00	70,98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gelatina, branca**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20206-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gelatina, branca

Special notes

When selecting the *Gelatina, branca* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gelatina, branca	3	3	34

Second-stage model

For differentiation of the substance/substance group *Gelatina, branca* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gelatina, branca* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	42,29	32,65
Cianocobalamina	74,37	37,64
⋮	⋮	⋮
Sulfato de colistina	>50	22,69
Bacitracina	>50	24,36
Anfotericina B	>50	44,52
Nistatina	>50	56,87
Pantotenato de cálcio	>50	59,53
Metilcobalamina	>50	70,81
Riboflavina	>50	75,37
Vitamina E acetato pó 50%	>50	81,43
Triancinolona	>50	93,10
Glicerofosfato de cálcio	>50	93,55
Carmelose sódica	>50	101,48
Levedura de selênio	>50	108,84
Bromidrato de hioscina	>50	112,63
Estradiol hemi-hidratado	>50	123,13
Tosilcloramida sódica	>50	134,02
Estriol	>50	141,15
SyrSpend® SF Alka	>50	150,01
Amido de arroz	>50	163,00
Ácido oxálico	>50	169,23
SyrSpend® SF pH4 neo	>50	181,51
SyrSpend® SF pH4	>50	195,23
Goma arábica, dispersão seca	>50	235,94
Amido de milho	>50	237,91
Fécula de batata	>50	290,73
Amido de trigo	>50	305,82
Maltodextrina	>50	318,99
Frutose	>50	326,18

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gelatina, branca* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gelatina, branca*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Gelatina, branca	11334025	20898	40	20111214
Caelo	Gelatina, branca	15320504	22499	40	AR-16-FG-014461-01
Caelo	Gelatina, branca	15320504	22582	45	AR-16-FG-011564-01
Caelo	Gelatina, branca	20000813	25289	40	20200417*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 165 spectra of 4 reference samples from the substance/substance group *Gelatina, branca*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 797 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Gelatina, branca*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Gelatina, branca	172772	23792	40
Caelo	Gelatina, branca	154419	23793	40
Caelo	Gelatina, branca	23002360	26943	40
Caelo	Gelatina, branca	23002360	26943SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 944 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 49 spectra from 32 *Apo-Ident* customers from 35 batches from the substance/substance group *Gelatina, branca*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gelatina, branca	2003763018	1
Caealo/Phoenix	Gelatina, branca	20003763003	2
Caelo	Gelatina, branca	11019308	1
Caelo	Gelatina, branca	11334020	1
Caelo	Gelatina, branca	11334025	4
Caelo	Gelatina, branca	12354401	1
Caelo	Gelatina, branca	12354507	3
Caelo	Gelatina, branca	14130901	2
Caelo	Gelatina, branca	14130912	1
Caelo	Gelatina, branca	15084801	1
Caelo	Gelatina, branca	15084806	1
Caelo	Gelatina, branca	15320502	2
Caelo	Gelatina, branca	15441902	1
Caelo	Gelatina, branca	1544191916	1
Caelo	Gelatina, branca	15441922	1
Caelo	Gelatina, branca	17277207	1
Caelo	Gelatina, branca	17277210	1
Caelo	Gelatina, branca	190907004	1
Caelo	Gelatina, branca	19090702	1
Caelo	Gelatina, branca	19090706	1
Caelo	Gelatina, branca	20003763001	1
Caelo	Gelatina, branca	20003763004	1
Caelo	Gelatina, branca	20003763006	1
Caelo	Gelatina, branca	20003763009	2
Caelo	Gelatina, branca	4110I-01578	1
Caelo	Gelatina, branca	8031701	1
Caelo	Gelatina, branca	8051811	1
Caesar & Loretz GmbH...	Gelatina, branca	20003763002	1
Caesar & Loretz GmbH...	Gelatina, branca	190907004	1
Caesar & Loretz GmbH	Gelatina, branca	17277208	1
Caesar & Loretz GmbH	Gelatina, branca	17277213	1
Caesar & Loretz GmbH	Gelatina, branca	190907001	1
Caesar & Loretz GmbH	Gelatina, branca	190907002	3
canea Pharma/noweda	Gelatina, branca	GR1617	1
EuRho / 20	Gelatina, branca	1106021-01	1
Euro OTC	Gelatina, branca	1106021-01	2
ROHA	Gelatina, branca	140110	1

- 236 018 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gelatina, branca* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gelatina, branca* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	165	0	152 797
Type B	0	140	0	201 944
Type C	0	49	0	236 018

The substance/substance group *Gelatina, branca* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.3636 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 87.7551 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20898	22582	9,12	95,36
22499	22499	0,00	94,01
22582	22582	0,00	90,86
25289	25289	0,00	97,72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glicerofosfato de cálcio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20352-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glicerofosfato de cálcio; Calcii glycerophosphas

Special notes

When selecting the *Glicerofosfato de cálcio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glicerofosfato de cálcio	7	4	70

Second-stage model

For differentiation of the substance/substance group *Glicerofosfato de cálcio* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glicerofosfato de cálcio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	45,29	–
Sulfato de polimixina B	46,82	17,33
⋮	⋮	⋮
Levedura de selênio	>50	20,18
Anfotericina B	>50	23,03
Sulfato de colistina	>50	23,22
Bacitracina	>50	34,79
SyrSpend® SF pH4 neo	>50	38,60
Pantotenato de cálcio	>50	39,23
Riboflavina	>50	46,49
Nistatina	>50	48,88
SyrSpend® SF Alka	>50	57,09
Carmelose sódica	>50	62,59
Amido de arroz	>50	66,91
Cianocobalamina	>50	71,40
Tosilcloramida sódica	>50	78,65
Gelatina, branca	>50	80,06
SyrSpend® SF pH4	>50	81,00
Estradiol hemi-hidratado	>50	83,46
Vitamina E acetato pó 50%	>50	85,43
Bromidrato de hioscina	>50	88,65
Triancinolona	>50	90,69
Metilcobalamina	>50	93,98
Goma arábica, dispersão seca	>50	94,65
Amido de milho	>50	94,71
Amido de trigo	>50	105,39
Ácido oxálico	>50	115,96
Fécula de batata	>50	120,87
Estriol	>50	130,27
Maltodextrina	>50	134,48
Frutose	>50	155,17

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glicerofosfato de cálcio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glicerofosfato de cálcio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glicerofosfato de cálcio	13007912	21311	40	20130124
Caelo	Glicerofosfato de cálcio	14341007	21969	60	AR-16-FG-005932-01
Caelo	Glicerofosfato de cálcio	191007	24538	40	20190502*
Caelo	Glicerofosfato de cálcio	20000551	25228	40	20200708*
Caelo	Glicerofosfato de cálcio	21000588	25634	40	20210217*
Fagron	Glicerofosfato de cálcio	13I17-N04	21234	40	20131016
Fagron	Glicerofosfato de cálcio	15B03-B03-305050	21978	60	1706313

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Glicerofosfato de cálcio*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Glicerofosfato de cálcio*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glicerofosfato de cálcio	12012411	20679	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glicerofosfato de cálcio	12012417	20771	40
Caelo	Glicerofosfato de cálcio	162310	23361	40
Caelo	Glicerofosfato de cálcio	20004507	26309	30
Caelo	Glicerofosfato de cálcio	20004507	26309SI	20

- 201 914 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 214 spectra from 127 *Apo-Ident* customers from 73 batches from the substance/substance group *Glicerofosfato de cálcio*.
- Among them are spectra of independent samples from 70 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Glicerofosfato de cálcio	B03-2224201	1
AHD	Glicerofosfato de cálcio	20004507016	1
AHD	Glicerofosfato de cálcio	20004507017	2
Caelo	Glicerofosfato de cálcio	12012406	1
Caelo	Glicerofosfato de cálcio	12012413	2
Caelo	Glicerofosfato de cálcio	13007902	1
Caelo	Glicerofosfato de cálcio	13007908	1
Caelo	Glicerofosfato de cálcio	13007912	2
Caelo	Glicerofosfato de cálcio	13007914	1
Caelo	Glicerofosfato de cálcio	13A18-N02	2
Caelo	Glicerofosfato de cálcio	13A18-No2	1
Caelo	Glicerofosfato de cálcio	14341007	5
Caelo	Glicerofosfato de cálcio	14341009	1
Caelo	Glicerofosfato de cálcio	14341010	1
Caelo	Glicerofosfato de cálcio	14341013	1
Caelo	Glicerofosfato de cálcio	14341015	1
Caelo	Glicerofosfato de cálcio	14347101	2
Caelo	Glicerofosfato de cálcio	14B10-B02-296841	1
Caelo	Glicerofosfato de cálcio	15B03B03305050	1
Caelo	Glicerofosfato de cálcio	15B03-B03-305050	1
Caelo	Glicerofosfato de cálcio	162310	1
Caelo	Glicerofosfato de cálcio	16231001	3
Caelo	Glicerofosfato de cálcio	16231004	3
Caelo	Glicerofosfato de cálcio	16231005	1
Caelo	Glicerofosfato de cálcio	16231006	4
Caelo	Glicerofosfato de cálcio	16231007	2
Caelo	Glicerofosfato de cálcio	16231008	2
Caelo	Glicerofosfato de cálcio	16231010	5
Caelo	Glicerofosfato de cálcio	17250703	5
Caelo	Glicerofosfato de cálcio	17359101	14
Caelo	Glicerofosfato de cálcio	17359101P-180122-1	1
Caelo	Glicerofosfato de cálcio	17359106	8
Caelo	Glicerofosfato de cálcio	17359107	9
Caelo	Glicerofosfato de cálcio	17359107P-181218-2	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicerofosfato de cálcio	17359110	1
Caelo	Glicerofosfato de cálcio	17359111	1
Caelo	Glicerofosfato de cálcio	180918A	1
Caelo	Glicerofosfato de cálcio	190762007	1
Caelo	Glicerofosfato de cálcio	191007001	3
Caelo	Glicerofosfato de cálcio	19100701	1
Caelo	Glicerofosfato de cálcio	19100702	5
Caelo	Glicerofosfato de cálcio	19100703	18
Caelo	Glicerofosfato de cálcio	19100707	5
Caelo	Glicerofosfato de cálcio	20000551002	1
Caelo	Glicerofosfato de cálcio	20000551003	4
Caelo	Glicerofosfato de cálcio	20004507001	2
Caelo	Glicerofosfato de cálcio	20004507004	3
Caelo	Glicerofosfato de cálcio	20004507005	1
Caelo	Glicerofosfato de cálcio	20004507007	2
Caelo	Glicerofosfato de cálcio	20004507014	2
Caelo	Glicerofosfato de cálcio	20004507016	2
Caelo	Glicerofosfato de cálcio	2004507001	1
Caelo	Glicerofosfato de cálcio	2004507017	1
Caesar & Loretz GmbH...	Glicerofosfato de cálcio	20004507017	1
Caesar & Loretz GmbH...	Glicerofosfato de cálcio	21000588001	2
Caesar & Loretz GmbH...	Glicerofosfato de cálcio	20004507001	2
Caesar & Loretz GmbH	Glicerofosfato de cálcio	191007001	2
Caesar & Loretz GmbH	Glicerofosfato de cálcio	19100703	1
Caesar & Loretz GmbH	Glicerofosfato de cálcio	19100707	1
Caesar & Loretz GmbH	Glicerofosfato de cálcio	20000551003	2
Caesar & Loretz GmbH	Glicerofosfato de cálcio	20004507001	2
Caesar & Loretz GmbH	Glicerofosfato de cálcio	20004507004	3
Caesar & Loretz GmbH	Glicerofosfato de cálcio	20004507007	3
Caesar & Loretz GmbH	Glicerofosfato de cálcio	20004507014	2
Caesar&Lorenz/AHD	Glicerofosfato de cálcio	16231010	1
Cealo/Sanacorp	Glicerofosfato de cálcio	17359101	1
Fagron	Glicerofosfato de cálcio	11G19-N05	1
Fagron	Glicerofosfato de cálcio	1216000005	1
Fagron	Glicerofosfato de cálcio	12I18-N06	3
Fagron	Glicerofosfato de cálcio	1314000019	1
Fagron	Glicerofosfato de cálcio	1317-N04	2
Fagron	Glicerofosfato de cálcio	13A18N02	2
Fagron	Glicerofosfato de cálcio	13A18-N02	5
Fagron	Glicerofosfato de cálcio	14B10B02	1
Fagron	Glicerofosfato de cálcio	14B10-B02	1
Fagron	Glicerofosfato de cálcio	14B10-B02-291642	1
Fagron	Glicerofosfato de cálcio	14B10-B02-296841	4
Fagron	Glicerofosfato de cálcio	15B03B03	1
Fagron	Glicerofosfato de cálcio	15B03-B03	1
Fagron	Glicerofosfato de cálcio	15B03-B03-305050	3
Fagron	Glicerofosfato de cálcio	17J17-B07-3583	1
Fagron	Glicerofosfato de cálcio	19J10-F06-366452	3
Fagron	Glicerofosfato de cálcio	2417Q-01212	1
Fagron	Glicerofosfato de cálcio	3115A-01212	1
Fagron	Glicerofosfato de cálcio	5212M-01212	1
Fagron	Glicerofosfato de cálcio	700338-0002	1
Gatt-Koller/Kwizda	Glicerofosfato de cálcio	4007/09123812	1
Gehe	Glicerofosfato de cálcio	16231006	1
Gehe	Glicerofosfato de cálcio	17359108	1
Gehe	Glicerofosfato de cálcio	19100701	2
Gehe	Glicerofosfato de cálcio	19100703	1
Gehe	Glicerofosfato de cálcio	20004507016	1
Phönix	Glicerofosfato de cálcio	20004507004	1
Sanacorp	Glicerofosfato de cálcio	16231008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Glicerofosfato de cálcio	17359102	1
Sanacorp	Glicerofosfato de cálcio	20000551002	1
Sanacorp	Glicerofosfato de cálcio	20004507007	1
Sidonia	Glicerofosfato de cálcio	17250703	1

- 235 853 spectra from 1515 *Apo-Ident* customers from a total of 49 186 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glicerofosfato de cálcio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glicerofosfato de cálcio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	170	0	201 914
Type C	0	214	0	235 853

The substance/substance group *Glicerofosfato de cálcio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.1963 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21234	21969	14,87	50,95
21311	21969	9,53	49,70

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21969	21969	0,00	50,81
21978	21978	0,00	46,94
24538	24538	0,00	46,85
25228	25228	0,00	42,94
25634	25634	0,00	44,94

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20823-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glicina; Glycinum

Special notes

When selecting the *Glicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glicina	11	16	15

Second-stage model

For differentiation of the substance/substance group *Glicina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
L-alanina	101,64	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glicina	13157303	21687	60	20130625
Caelo	Glicina	14147006	21818	60	AR-16-FG-012263-01
Caelo	Glicina	15262518	23124	40	20150910
Caelo	Glicina	170265	23295	40	20170315*
Caelo	Glicina	173493	23834	40	20180117*
Caelo	Glicina	20001656	25218	40	20200703*
Caelo	Glicina	22002518	26368	40	20220926*
Caelo	Glicina	22002518	26368SI	20	20220926*
Euro OTC	Glicina	1402022-01	21284	40	20140328
Euro OTC	Glicina	1402022-01	21534	60	AR-15-FG-005430-01
Euro OTC	Glicina	1801005	23912	40	20180125*
Fagron	Glicina	12G13-N04	20823	40	1401163
Fagron	Glicina	13G09-N03	21276	40	20120711

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 560 spectra of 13 reference samples from the substance/substance group *Glicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 402 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 710 spectra of 20 reference samples from the substance/substance group *Glicina*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glicina	191009	24507	40
Caelo	Glicina	23002306	26957	40
Caelo	Glicina	24001068	27319	40
Euro OTC	Glicina	1605035	22683	40
Euro OTC	Glicina	1704015	23387	40
Euro OTC	Glicina	1906006	24793	40
Euro OTC	Glicina	1911011	25103	40
Euro OTC	Glicina	2005028	25291	40
Euro OTC	Glicina	2009013	25424	40
Euro OTC	Glicina	2101030	25529	40
Euro OTC	Glicina	2203024	26038	40
Euro OTC	Glicina	2301025	26647	40
Euro OTC	Glicina	2307011	26890	40
Euro OTC	Glicina	2307010	26891	40
Euro OTC	Glicina	2404013	27364	40
Fagron	Glicina	23G05-B12-230974	26987	40
Caelo	Glicina	24001068	27319SI	20
Euro OTC	Glicina	2203024	26038SI	10
Euro OTC	Glicina	2301025	26647SI	20
Euro OTC	Glicina	2404013	27364SI	20

- 201 374 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

provided by the customer regarding manufacturer and batch number.

- 31 spectra from 13 *Apo-Ident* customers from 16 batches from the substance/substance group *Glicina*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Glicina	14147005	1
Caelo	Glicina	15262502	2
Caelo	Glicina	15262503	1
Caelo	Glicina	15262504	1
Caelo	Glicina	15262518	1
Caelo	Glicina	17026502	1
Caelo	Glicina	19100902	3
Caesar & Loretz GmbH	Glicina	17349306	1
Caesar & Loretz GmbH	Glicina	19100902	2
Caesar & Loretz GmbH	Glicina	19100903	2
Euro OTC	Glicina	1801005-01	1
Euro OTC	Glicina	1906006-01	1
Euro OTC	Glicina	2101030-01	4
Euro OTC	Glicina	2203024-01	3
Fagron	Glicina	19E29-B04-366853	1
Fagron	Glicina	20J13-F06-374988	1
Fagron	Glicina	20J13-F06-376061	4
Sanacorp	Glicina	17349306	1

- 236 036 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	560	0	152 402
Type B	0	710	0	201 374
Type C	0	31	0	236 036

The substance/substance group *Glicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9286 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1549 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 80.6452 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20823	20823	0,00	196,73
21276	20823	13,50	198,73
21284	21534	13,20	182,97
21534	21534	0,00	179,85
21687	21534	15,31	184,83
21818	21818	0,00	213,08
23124	20823	31,44	193,55
23295	23295	0,00	210,67
23834	23834	0,00	184,08
23912	23912	0,00	181,20
25218	25218	0,00	205,90
26368	26368	0,00	183,62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glicose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20982-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glicose; Glucosum

Special notes

When selecting the *Glicose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glicose	6	2	250

Second-stage model

For differentiation of the substance/substance group *Glicose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glicose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	84,70	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glicose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glicose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glicose	12294514	20982	40	1402475
Caelo	Glicose	14033901	21363	40	20140214
Caelo	Glicose	14142310	21703	45	20140523
Caelo	Glicose	16050501	22586	40	20160317
Caelo	Glicose	190380	24511	40	20190411*
Caelo	Glicose	22002306	26366	40	20220909*
Caelo	Glicose	22002306	26366SI	20	20220909*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 265 spectra of 7 reference samples from the substance/substance group *Glicose*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 697 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Glicose*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glicose	16157401	23583	40
Caelo	Glicose	180129	23820	40

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1521 spectra from 309 *Apo-Ident* customers from 257 batches from the substance/substance group *Glicose*.
- Among them are spectra of independent samples from 249 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Glicose		1
	Glicose	21002549009	1
	Glicose	21002549010	1
	Glicose	21002549012	7
	Glicose	21002549014	1
	Glicose	22002306002	1
	Glicose	22002306003	2
	Glicose	22002306006	10
	Glicose	22002306008	1
	Glicose	22002306010	2
	Glicose	22003206006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
21.03.2017	Glicose	6910499	1
AHD	Glicose	14033908	1
AHD	Glicose	21002549004	1
AHD	Glicose	21002549014	1
AHD	Glicose	22002306010	1
Aliance Healthcare	Glicose	21002549012	2
Allianc. Healthc. /c	Glicose	16050510	1
Anzag	Glicose	13329505	1
Apotheke/Defektur Mi...	Glicose		1
Apotheke-SiO2-Mischung	Glicose	18/15	1
Audor Pharma	Glicose	16157402	3
Bombastus	Glicose	160505202	1
Caelo	Glicose	1001313393	1
Caelo	Glicose	10091503	1
Caelo	Glicose	1061703	1
Caelo	Glicose	106213393	1
Caelo	Glicose	1114A03393	1
Caelo	Glicose	11358823	1
Caelo	Glicose	12041801	1
Caelo	Glicose	120718A	1
Caelo	Glicose	12141705	1
Caelo	Glicose	12141706	3
Caelo	Glicose	12141714	2
Caelo	Glicose	12141715	1
Caelo	Glicose	12141717	1
Caelo	Glicose	12141718	3
Caelo	Glicose	12294505	3
Caelo	Glicose	12294509	2
Caelo	Glicose	12294509-3425311150	1
Caelo	Glicose	12294510	3
Caelo	Glicose	12294511	1
Caelo	Glicose	12294514	2
Caelo	Glicose	12294515	2
Caelo	Glicose	12294517	1
Caelo	Glicose	12294519	1
Caelo	Glicose	13041501	1
Caelo	Glicose	1317815	1
Caelo	Glicose	13178701	2
Caelo	Glicose	13178702	1
Caelo	Glicose	13178704	3
Caelo	Glicose	13178707	2
Caelo	Glicose	13178711	2
Caelo	Glicose	13178712	1
Caelo	Glicose	13178715	4
Caelo	Glicose	13178716	1
Caelo	Glicose	13178718	1
Caelo	Glicose	13329501	3
Caelo	Glicose	13329503	3
Caelo	Glicose	13329504	2
Caelo	Glicose	13329507	1
Caelo	Glicose	13329512	7
Caelo	Glicose	14033901	2
Caelo	Glicose	14033902	4
Caelo	Glicose	14033906	5
Caelo	Glicose	14033907	5
Caelo	Glicose	14033908	2
Caelo	Glicose	14051401	1
Caelo	Glicose	14051802	1
Caelo	Glicose	14142301	1
Caelo	Glicose	14142303	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose	14142304	1
Caelo	Glicose	14142308	1
Caelo	Glicose	14142310	5
Caelo	Glicose	14142313	2
Caelo	Glicose	14142314	3
Caelo	Glicose	1415U-03393	1
Caelo	Glicose	14319302	1
Caelo	Glicose	14319304	6
Caelo	Glicose	14319308	1
Caelo	Glicose	14319309	3
Caelo	Glicose	14319310	2
Caelo	Glicose	1439304	1
Caelo	Glicose	15021801	1
Caelo	Glicose	15051301	1
Caelo	Glicose	15081831	1
Caelo	Glicose	1509500	3
Caelo	Glicose	15095001	8
Caelo	Glicose	15095003	4
Caelo	Glicose	15095004	3
Caelo	Glicose	15095005	2
Caelo	Glicose	15148801	4
Caelo	Glicose	15148802	6
Caelo	Glicose	15148803	1
Caelo	Glicose	15148807	4
Caelo	Glicose	15148808	4
Caelo	Glicose	15148809	1
Caelo	Glicose	15148810	4
Caelo	Glicose	15148813	1
Caelo	Glicose	15329001	6
Caelo	Glicose	15329002	2
Caelo	Glicose	15329004	4
Caelo	Glicose	15329005	4
Caelo	Glicose	15329006	11
Caelo	Glicose	15329008	2
Caelo	Glicose	15329010	2
Caelo	Glicose	160308G	1
Caelo	Glicose	16050501	19
Caelo	Glicose	16050502	12
Caelo	Glicose	16050503	23
Caelo	Glicose	16050504	1
Caelo	Glicose	16050507	3
Caelo	Glicose	16050508	3
Caelo	Glicose	16050510	3
Caelo	Glicose	16101204	1
Caelo	Glicose	16101205	1
Caelo	Glicose	1614U3393	1
Caelo	Glicose	16157402	5
Caelo	Glicose	16157403	28
Caelo	Glicose	16157403160117/1	1
Caelo	Glicose	16157406	24
Caelo	Glicose	16157406160117/2	1
Caelo	Glicose	16157411	10
Caelo	Glicose	16328801	16
Caelo	Glicose	16328803	14
Caelo	Glicose	16328805	21
Caelo	Glicose	16328807	6
Caelo	Glicose	16328811	9
Caelo	Glicose	16328812	16
Caelo	Glicose	16328813	1
Caelo	Glicose	1638803	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose	1650502	1
Caelo	Glicose	17041701	1
Caelo	Glicose	17111803	1
Caelo	Glicose	18012902	31
Caelo	Glicose	1801290246/18	1
Caelo	Glicose	18012903	3
Caelo	Glicose	18012905	13
Caelo	Glicose	18012907	39
Caelo	Glicose	18012909	14
Caelo	Glicose	18012910	2
Caelo	Glicose	18012911	6
Caelo	Glicose	18012912	29
Caelo	Glicose	18012913	8
Caelo	Glicose	18012914	17
Caelo	Glicose	18012915	26
Caelo	Glicose	18012916	1
Caelo	Glicose	18012917	10
Caelo	Glicose	18012920	4
Caelo	Glicose	18012921	36
Caelo	Glicose	18012922	7
Caelo	Glicose	18012923	3
Caelo	Glicose	18012926	3
Caelo	Glicose	18111702	1
Caelo	Glicose	1812913	1
Caelo	Glicose	19028005	1
Caelo	Glicose	190320011	1
Caelo	Glicose	190380002	5
Caelo	Glicose	190380003	40
Caelo	Glicose	190380006	8
Caelo	Glicose	190380007	1
Caelo	Glicose	190380009	32
Caelo	Glicose	19038001	7
Caelo	Glicose	190380011	2
Caelo	Glicose	19038002	45
Caelo	Glicose	19038003	6
Caelo	Glicose	19038005	12
Caelo	Glicose	19038006	14
Caelo	Glicose	19038007	42
Caelo	Glicose	19080009	2
Caelo	Glicose	1914I03393	1
Caelo	Glicose	20001066020	2
Caelo	Glicose	20004066	1
Caelo	Glicose	20004066001	5
Caelo	Glicose	20004066002	3
Caelo	Glicose	20004066004	31
Caelo	Glicose	200040660042x	1
Caelo	Glicose	20004066005	4
Caelo	Glicose	200040660058	1
Caelo	Glicose	20004066006	6
Caelo	Glicose	20004066008	49
Caelo	Glicose	20004066010	8
Caelo	Glicose	20004066011	5
Caelo	Glicose	20004066013	1
Caelo	Glicose	20004066014	1
Caelo	Glicose	20004066015	6
Caelo	Glicose	20004066017	7
Caelo	Glicose	20004066018	19
Caelo	Glicose	20004066019	1
Caelo	Glicose	20004066020	4
Caelo	Glicose	20004066021	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose	20004066023	12
Caelo	Glicose	2000406608	1
Caelo	Glicose	2000406611	1
Caelo	Glicose	2004066008	1
Caelo	Glicose	2004066014	1
Caelo	Glicose	2004066021	1
Caelo	Glicose	2004066023	1
Caelo	Glicose	200406604	1
Caelo	Glicose	2013Q-03393	1
Caelo	Glicose	2021902	1
Caelo	Glicose	2051701	1
Caelo	Glicose	208223393	1
Caelo	Glicose	210002549007	1
Caelo	Glicose	210002549012	1
Caelo	Glicose	2100254009	1
Caelo	Glicose	21002549	1
Caelo	Glicose	21002549002	2
Caelo	Glicose	21002549003	29
Caelo	Glicose	21002549004	8
Caelo	Glicose	21002549007	23
Caelo	Glicose	21002549008	2
Caelo	Glicose	21002549009	6
Caelo	Glicose	21002549012	17
Caelo	Glicose	21002549013	3
Caelo	Glicose	21002549014	1
Caelo	Glicose	2102201301	1
Caelo	Glicose	214U-03393	1
Caelo	Glicose	220002306003	1
Caelo	Glicose	23091401	1
Caelo	Glicose	250004066021	1
Caelo	Glicose	25061204	1
Caelo	Glicose	2513M03393	1
Caelo	Glicose	26041303	1
Caelo	Glicose	28111714	1
Caelo	Glicose	2x18012915	1
Caelo	Glicose	3121402	1
Caelo	Glicose	3214M-03393	1
Caelo	Glicose	3513I-03393	1
Caelo	Glicose	3918M-03393	1
Caelo	Glicose	402313393	2
Caelo	Glicose	4071505	1
Caelo	Glicose	4117I-03393	1
Caelo	Glicose	4313Q3393	1
Caelo	Glicose	4616I-03393	1
Caelo	Glicose	4713l-03393	1
Caelo	Glicose	5013I3393	1
Caelo	Glicose	5081401	1
Caelo	Glicose	551616157406	1
Caelo	Glicose	6031505	1
Caelo	Glicose	6071717	1
Caelo	Glicose	69010513	1
Caelo	Glicose	7091705	1
Caelo	Glicose	712213393	1
Caelo	Glicose	8031703	1
Caelo	Glicose	8091810	1
Caelo	Glicose	85(06910499)	1
Caelo	Glicose	AKD14	1
Caelo	Glicose	I-180716-1605010	1
Caesar & Loretz GmbH...	Glicose	20004066018	2
Caesar & Loretz GmbH...	Glicose	20004066008	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Glicose	21002549005	1
Caesar & Loretz GmbH...	Glicose	20004066023	2
Caesar & Loretz GmbH...	Glicose	21002549009	1
Caesar & Loretz GmbH...	Glicose	20004066006	3
Caesar & Loretz GmbH/Gehe	Glicose	190380003	3
Caesar & Loretz GmbH/Gehe	Glicose	20004066011	1
Caesar & Loretz GmbH/Gehe	Glicose	21002549007	1
Caesar & Loretz GmbH...	Glicose	19038002	2
Caesar & Loretz GmbH...	Glicose	21002549003	1
Caesar & Loretz GmbH...	Glicose	190380009	1
Caesar & Loretz GmbH...	Glicose	20004066013	1
Caesar & Loretz GmbH...	Glicose	20004066017	1
Caesar & Loretz GmbH...	Glicose	21002549003	4
Caesar & Loretz GmbH...	Glicose	19038002	1
Caesar & Loretz GmbH...	Glicose	21002549003	1
Caesar & Loretz GmbH	Glicose	16157403	1
Caesar & Loretz GmbH	Glicose	18012909	1
Caesar & Loretz GmbH	Glicose	18012912	1
Caesar & Loretz GmbH	Glicose	18012915	2
Caesar & Loretz GmbH	Glicose	18012921	10
Caesar & Loretz GmbH	Glicose	18012922	2
Caesar & Loretz GmbH	Glicose	18012926	1
Caesar & Loretz GmbH	Glicose	190380002	4
Caesar & Loretz GmbH	Glicose	190380003	7
Caesar & Loretz GmbH	Glicose	190380005	1
Caesar & Loretz GmbH	Glicose	190380009	5
Caesar & Loretz GmbH	Glicose	19038001	3
Caesar & Loretz GmbH	Glicose	190380010	2
Caesar & Loretz GmbH	Glicose	19038002	1
Caesar & Loretz GmbH	Glicose	19038005	2
Caesar & Loretz GmbH	Glicose	19038006	1
Caesar & Loretz GmbH	Glicose	19038007	5
Caesar & Loretz GmbH	Glicose	20004066002	3
Caesar & Loretz GmbH	Glicose	20004066004	2
Caesar & Loretz GmbH	Glicose	20004066005	2
Caesar & Loretz GmbH	Glicose	20004066007	1
Caesar & Loretz GmbH	Glicose	20004066008	2
Caesar & Loretz GmbH	Glicose	20004066010	1
Caesar & Loretz GmbH	Glicose	20004066011	1
Caesar & Loretz GmbH	Glicose	20004066017	1
Caesar & Loretz GmbH	Glicose	20004066018	1
Caesar & Loretz GmbH	Glicose	20004066020	2
Caesar & Loretz GmbH	Glicose	20004066022	1
Caesar & Loretz GmbH	Glicose	21002549002	3
Caesar & Loretz GmbH	Glicose	21002549003	3
Caesar & Loretz GmbH	Glicose	21002549004	1
Caesar & Loretz GmbH	Glicose	21002549007	3
Caesar & Loretz GmbH	Glicose	21002549008	2
Caesar & Loretz GmbH	Glicose	21002549009	1
Caesar & Loretz GmbH	Glicose	21002549012	2
Caesar & Loretz GmbH	Glicose	21002549013	1
Caesar & Loretz GmbH	Glicose	21002549014	1
Caesar & Loretz GmbH	Glicose	210025949007	1
Caesar & Loretz Hild...	Glicose	18012921	1
Caesar & Loretz Hild...	Glicose	190380003	2
Caesar & Loretz Hild...	Glicose	190380003190380009	1
Caesar & Loretz Hild...	Glicose	19038007	1
Caesar & Loretz Hilden	Glicose	18012914	2
Caesar & Loretz Hilden	Glicose	18012915	1
Caesar & Loretz Hilden	Glicose	19038002	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz Hilden	Glicose	20004066004	1
Caesar & Loretz/ Pho…	Glicose	20004066004	2
Caesar & Loretz	Glicose	16157402	1
Caesar & Loretz	Glicose	18012923	1
Caesar u. Loretz GmbH	Glicose	190380003	2
Caesar u. Loretz GmbH	Glicose	190380009	1
Caesar u. Loretz GmbH	Glicose	20004066008	2
Caesar&Loretz GmbH	Glicose	19038006	3
Caesar&loretz,Anzag	Glicose	12294509	1
Caesar&Loretz	Glicose	15148808	1
Euro OTC	Glicose		1
Euro OTC	Glicose	15148808	1
Euro OTC	Glicose	16050501	1
Euro OTC	Glicose	16050502	2
Euro OTC	Glicose	18012905	3
Euro OTC	Glicose	18012922	1
Fagron	Glicose	13178716	1
Fagron	Glicose	14142303	1
Fagron	Glicose	15329005	2
Fiebig 02.05.2019	Glicose	18012915	1
Fiebig	Glicose	18012907	1
GEHE 17.07.2014	Glicose	14033907	1
Gehe 27.11.14	Glicose	14142309	1
Gehe Kassel	Glicose	14142313	1
GEHE	Glicose	13178715	1
Gehe	Glicose	16157403	2
GEHE	Glicose	16157406	1
GEHE	Glicose	16328801	1
Gehe	Glicose	16328803	1
Gehe	Glicose	16328805	4
GEHE	Glicose	16328805	1
Gehe	Glicose	163288205	1
Gehe	Glicose	18012902	1
GEHE	Glicose	18012902	2
Gehe	Glicose	18012907	2
GEHE	Glicose	18012907	4
Gehe	Glicose	18012912	1
GEHE	Glicose	18012912	2
Gehe	Glicose	18012914	1
Gehe	Glicose	18012915	2
GEHE	Glicose	18012915	4
Gehe	Glicose	18012921	2
Gehe	Glicose	190380003	7
GEHE	Glicose	19038002	2
Gehe	Glicose	19038003	1
Gehe	Glicose	19038007	1
Gehe	Glicose	20004066004	2
gehe	Glicose	22002306003	1
Geibo/Noweda	Glicose	18012907	1
Geibo	Glicose	190380003	1
Geibo	Glicose	19038007	2
Geilenkirchen	Glicose	18012902	1
Geilenkirchen	Glicose	18012921	3
Geilenkirchen	Glicose	190380009	1
Geilenkirchen	Glicose	20004066023	1
Ichtyol-Ges HH/Sanacorp	Glicose	18012909	1
Jenne	Glicose	12141705	1
Klenk	Glicose	16050502	1
Max Jenne	Glicose	23002088001	1
Nachprüfung	Glicose		2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Glicose	18012922	1
Noweda	Glicose	20004066004	1
Noweda	Glicose	20004066014	1
Noweda	Glicose	21002549007	4
Noweda	Glicose	21002549008	1
PHOENIX 30.05.2014	Glicose	13329514	1
PHOENIX 30.05.2014	Glicose	14033902	1
Phoenix	Glicose	14142310	1
Phoenix	Glicose	15148801	1
Phoenix	Glicose	15329010	2
Phoenix	Glicose	16050501	1
Phoenix	Glicose	16050503	4
Phoenix	Glicose	190380009	1
Phoenix	Glicose	191250611	1
Phönix/Fagon	Glicose	16328807	1
Phönix	Glicose	13178701	1
PHÖNIX	Glicose	16328812	3
PHÖNIX	Glicose	18012902	1
Rondell Apotheke	Glicose	15329003	1
Sanacorp	Glicose	12294509	1
Sanacorp	Glicose	16328805	1
Sanacorp	Glicose	18012907	2
Sanacorp	Glicose	18012909	1
Sanacorp	Glicose	190380009	2
Sanacorp	Glicose	20004066023	1
Sanacorp	Glicose	2004066023	1
Sanacorp	Glicose	21002549008	1
sanacorp	Glicose	22002306003	1
Sanacorp	Glicose	22002306003	1
Sanacorp	Glicose	22002306006	4
Sanacorp	Glicose	23002088001	1
Sonnen-Apotheke Wefe…	Glicose	17/16	1
Sonnen-Apotheke Wefe…	Glicose	21/17Glucose-SiO2-M	1
Sonnen-Apotheke Wefe…	Glicose	34/16	1

- 234 546 spectra from 1515 *Apo-Ident* customers from a total of 49 003 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glicose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glicose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	265	0	152 697
Type B	0	80	0	202 004
Type C	0	1518	3	234 546

The substance/substance group *Glicose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7358 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	99.8028 % (> 99.6055 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20982	20982	0,00	218,11
21363	26366	10,79	227,54
21703	20982	6,16	222,64
22586	20982	4,10	222,40
24511	24511	0,00	238,58
26366	26366	0,00	244,18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glicose monoidratada**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20031-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glicose monoidratada; Glucosum monohydricum

Special notes

When selecting the *Glicose monoidratada* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glicose monoidratada	12	23	566

Second-stage model

For differentiation of the substance/substance group *Glicose monoidratada* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glicose monoidratada* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	78,17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glicose monoidratada* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glicose monoidratada*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glicose monoidratada	171368	23304	40	20170601*
Caelo	Glicose monoidratada	173050	23802	40	20171110*
Caelo	Glicose monoidratada	20003964	25627	40	20210115*
Caelo	Glicose monoidratada	20003963	25637	40	20210115*
Caelo	Glicose monoidratada	20002144	25653	40	20200813*
Euro OTC	Glicose monoidratada	1509006	21905	60	20150914*
Euro OTC	Glicose monoidratada	1601016	22308	60	20160129*
Euro OTC	Glicose monoidratada	1604006	22538	40	20160511*
Euro OTC	Glicose monoidratada	1701002	23006	40	20170213*
Euro OTC	Glicose monoidratada	1807005	24162	40	20180718*
Fagron	Glicose monoidratada	11L19-N13	20799	40	20120105
Fagron	Glicose monoidratada	14B04-B01	21274	40	20140304

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 520 spectra of 12 reference samples from the substance/substance group *Glicose monoidratada*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 442 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 970 spectra of 26 reference samples from the substance/substance group *Glicose monoidratada*.

- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glicose monoidratada	16184807	23025	40
Caelo	Glicose monoidratada	190733	24506	40
Caelo	Glicose monoidratada	182174	24906	40
Caelo	Glicose monoidratada	22001899	26364	30
Caelo	Glicose monoidratada	24002353	27438	40
Euro OTC	Glicose monoidratada	1210034-02	21285	40
Euro OTC	Glicose monoidratada	1607024	22692	40
Euro OTC	Glicose monoidratada	1707004	23545	40
Euro OTC	Glicose monoidratada	1801009	23897	40
Euro OTC	Glicose monoidratada	1811020	24418	40
Euro OTC	Glicose monoidratada	1904029	24640	40
Euro OTC	Glicose monoidratada	1908012	24860	40
Euro OTC	Glicose monoidratada	2001006	25083	40
Euro OTC	Glicose monoidratada	2006007	25310	40
Euro OTC	Glicose monoidratada	2009024	25461	40
Euro OTC	Glicose monoidratada	2103027	25671	40
Euro OTC	Glicose monoidratada	2107024	25772	50
Euro OTC	Glicose monoidratada	2109008	25824	50
Euro OTC	Glicose monoidratada	2202015	26040	40
Euro OTC	Glicose monoidratada	2206018	26209	40
Euro OTC	Glicose monoidratada	2210005	26418	30
Euro OTC	Glicose monoidratada	2302007	26591	40
Euro OTC	Glicose monoidratada	2310008	26997	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glicose monoidratada	22001899	26364SI	20
Euro OTC	Glicose monoidratada	2202015	26040SI	10
Euro OTC	Glicose monoidratada	2206018	26209SI	20

- 201 114 spectra from a total of 4022 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4533 spectra from 906 *Apo-Ident* customers from 575 batches from the substance/substance group *Glicose monoidratada*.

- Among them are spectra of independent samples from 566 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Glicose monoidratada		2
	Glicose monoidratada	21001886009	1
	Glicose monoidratada	2109008-01	1
	Glicose monoidratada	2109008-02	1
	Glicose monoidratada	22000756006	3
	Glicose monoidratada	22000756007	1
	Glicose monoidratada	22000756015	1
	Glicose monoidratada	22000756019	8
	Glicose monoidratada	22000756021	1
	Glicose monoidratada	22001899002	12
	Glicose monoidratada	22001899003	2
	Glicose monoidratada	22001899005	5
	Glicose monoidratada	22001899010	2
	Glicose monoidratada	22001899011	13
	Glicose monoidratada	2200756015	1
	Glicose monoidratada	2202015-03	1
	Glicose monoidratada	22021899011	1
	Glicose monoidratada	2206018-01	3
	Glicose monoidratada	2206018-02	1
	Glicose monoidratada	2210005-01	3
	Glicose monoidratada	221000502	1
	Glicose monoidratada	2210005-02	6
	Glicose monoidratada	23000211001	2
	Glicose monoidratada	23000211002	1
	Glicose monoidratada	23000211004	1
	Glicose monoidratada	23000211005	9
	Glicose monoidratada	23000211006	2
	Glicose monoidratada	23000211010	2
	Glicose monoidratada	230008-01	1
	Glicose monoidratada	23003430002	1
	Glicose monoidratada	2302007-01	10
	Glicose monoidratada	2302007-02	4
	Glicose monoidratada	23100008-02	1
	Glicose monoidratada	2310008-01	6
	Glicose monoidratada	24000422002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Glicose monoidratada	24000422004	1
	Glicose monoidratada	24000422005	1
	Glicose monoidratada	557473	1
73098/Gehe	Glicose monoidratada	E388S	1
ACM	Glicose monoidratada	KNC1164J15	1
ACM	Glicose monoidratada	KNC1282J14	1
AHD	Glicose monoidratada	14102407	1
AHD	Glicose monoidratada	21001886013	1
AHD	Glicose monoidratada	2202015-02	1
AHD	Glicose monoidratada	2210005-01	2
AHD	Glicose monoidratada	2310008-01	2
AHD	Glicose monoidratada	24000422004	1
Alliance/EurRho	Glicose monoidratada	2103027-01	1
Alliance	Glicose monoidratada	16049101	1
Alliance	Glicose monoidratada	22000756011	1
Alliance	Glicose monoidratada	22001899005	1
Alliance	Glicose monoidratada	2202015-02	1
Allianz Healthcare	Glicose monoidratada	19073305	1
allianz	Glicose monoidratada	1543409	1
Anzag	Glicose monoidratada	14334810	1
Anzag	Glicose monoidratada	16184808	1
Anzag	Glicose monoidratada	17005804	1
Anzag	Glicose monoidratada	17136805	1
api-ident / AHD	Glicose monoidratada	2009024-01	1
apo ident/Noweda	Glicose monoidratada	2103027-01	1
apo ident	Glicose monoidratada	202015-02	1
Apoident/ Phoenix	Glicose monoidratada	2009024-01	1
Apo-Ident/Phoenix	Glicose monoidratada	1701002-01	1
Apo-Ident/Phoenix	Glicose monoidratada	1707004-01	3
apo-ident	Glicose monoidratada	1604006-02	1
ApoIdent	Glicose monoidratada	2107024-02	1
ApoIdent	Glicose monoidratada	2206018-01	1
Apotheke im Forum	Glicose monoidratada	17010002-01	1
Audor Pharma	Glicose monoidratada	2202015-03	1
Audor Pharma	Glicose monoidratada	2206018-01	2
Audor Pharma	Glicose monoidratada	E732N	1
Beiersdorf/Phönix	Glicose monoidratada	L6209	1
Bombastus	Glicose monoidratada	14334802	2
Bombastus	Glicose monoidratada	15413410	1
Bombastus	Glicose monoidratada	16184810	2
Bombastus	Glicose monoidratada	1807005-01	1
Bombastus	Glicose monoidratada	18101901	2
Bombastus	Glicose monoidratada	18214703	3
Caello/Phönix	Glicose monoidratada	15095601	3
Caelo	Glicose monoidratada		3
Caelo	Glicose monoidratada	10159501	1
Caelo	Glicose monoidratada	1073303	1
Caelo	Glicose monoidratada	11021509	1
Caelo	Glicose monoidratada	11082014	1
Caelo	Glicose monoidratada	11082020	1
Caelo	Glicose monoidratada	111111111	1
Caelo	Glicose monoidratada	11314516	3
Caelo	Glicose monoidratada	11314519	1
Caelo	Glicose monoidratada	11314526	1
Caelo	Glicose monoidratada	11314528	8
Caelo	Glicose monoidratada	1134506	1
Caelo	Glicose monoidratada	11L19-N13	3
Caelo	Glicose monoidratada	1204044-01	2
Caelo	Glicose monoidratada	12284202	6
Caelo	Glicose monoidratada	12284204	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose monoidratada	12284206	6
Caelo	Glicose monoidratada	12284219	8
Caelo	Glicose monoidratada	12284222	3
Caelo	Glicose monoidratada	12284229	3
Caelo	Glicose monoidratada	12284230	3
Caelo	Glicose monoidratada	12284231	1
Caelo	Glicose monoidratada	12345	1
Caelo	Glicose monoidratada	123456	2
Caelo	Glicose monoidratada	12435	1
Caelo	Glicose monoidratada	12G30-N01	1
Caelo	Glicose monoidratada	12G30-NO01	1
Caelo	Glicose monoidratada	1305030-02	1
Caelo	Glicose monoidratada	13157002	2
Caelo	Glicose monoidratada	13157004	1
Caelo	Glicose monoidratada	13157005	12
Caelo	Glicose monoidratada	13157007	6
Caelo	Glicose monoidratada	13157008	1
Caelo	Glicose monoidratada	13157011	9
Caelo	Glicose monoidratada	13157012	1
Caelo	Glicose monoidratada	13157013	1
Caelo	Glicose monoidratada	13157017	1
Caelo	Glicose monoidratada	13157019	10
Caelo	Glicose monoidratada	13157022	1
Caelo	Glicose monoidratada	13157026	3
Caelo	Glicose monoidratada	13A25-N01	5
Caelo	Glicose monoidratada	13H06-N08	2
Caelo	Glicose monoidratada	1410019-02	1
Caelo	Glicose monoidratada	14102401	4
Caelo	Glicose monoidratada	14102407	2
Caelo	Glicose monoidratada	14102411	4
Caelo	Glicose monoidratada	14102412	9
Caelo	Glicose monoidratada	14102415	2
Caelo	Glicose monoidratada	14102416	5
Caelo	Glicose monoidratada	14102418	10
Caelo	Glicose monoidratada	14102420	6
Caelo	Glicose monoidratada	14102421	4
Caelo	Glicose monoidratada	14102424	1
Caelo	Glicose monoidratada	14102427	1
Caelo	Glicose monoidratada	14102430	3
Caelo	Glicose monoidratada	14334802	11
Caelo	Glicose monoidratada	14334805	2
Caelo	Glicose monoidratada	14334806	3
Caelo	Glicose monoidratada	14334807	4
Caelo	Glicose monoidratada	14334808	2
Caelo	Glicose monoidratada	14334809	1
Caelo	Glicose monoidratada	14334810	8
Caelo	Glicose monoidratada	14334811	2
Caelo	Glicose monoidratada	14B04-B01-291137	1
Caelo	Glicose monoidratada	14B28-B02-291354	1
Caelo	Glicose monoidratada	14I04-B08	4
Caelo	Glicose monoidratada	150302G	1
Caelo	Glicose monoidratada	15095601	9
Caelo	Glicose monoidratada	15095602	1
Caelo	Glicose monoidratada	15095603	1
Caelo	Glicose monoidratada	15095605	3
Caelo	Glicose monoidratada	15095606	1
Caelo	Glicose monoidratada	15095611	3
Caelo	Glicose monoidratada	15095612	13
Caelo	Glicose monoidratada	15180001	12
Caelo	Glicose monoidratada	15180002	17

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose monoidratada	15180003	3
Caelo	Glicose monoidratada	15180005	3
Caelo	Glicose monoidratada	15180009	1
Caelo	Glicose monoidratada	15180010	8
Caelo	Glicose monoidratada	15180012	18
Caelo	Glicose monoidratada	15180013	2
Caelo	Glicose monoidratada	15180015	8
Caelo	Glicose monoidratada	15180016	2
Caelo	Glicose monoidratada	1518002	1
Caelo	Glicose monoidratada	15413301	1
Caelo	Glicose monoidratada	15413302	3
Caelo	Glicose monoidratada	15413303	1
Caelo	Glicose monoidratada	15413304	27
Caelo	Glicose monoidratada	15413304/20160309/6	1
Caelo	Glicose monoidratada	15413401	6
Caelo	Glicose monoidratada	15413402	6
Caelo	Glicose monoidratada	15413405	6
Caelo	Glicose monoidratada	15413409	25
Caelo	Glicose monoidratada	15413410	3
Caelo	Glicose monoidratada	15413412	3
Caelo	Glicose monoidratada	15413413	1
Caelo	Glicose monoidratada	154134o2	1
Caelo	Glicose monoidratada	160101	1
Caelo	Glicose monoidratada	160400601	1
Caelo	Glicose monoidratada	1604006-01	1
Caelo	Glicose monoidratada	1604104	1
Caelo	Glicose monoidratada	16049101	19
Caelo	Glicose monoidratada	16049102	9
Caelo	Glicose monoidratada	16049103	6
Caelo	Glicose monoidratada	16049104	19
Caelo	Glicose monoidratada	16049105	10
Caelo	Glicose monoidratada	16049107	6
Caelo	Glicose monoidratada	16049108	4
Caelo	Glicose monoidratada	1607024-01	1
Caelo	Glicose monoidratada	1618401	2
Caelo	Glicose monoidratada	16184616	1
Caelo	Glicose monoidratada	16184801	20
Caelo	Glicose monoidratada	16184802	2
Caelo	Glicose monoidratada	16184807	12
Caelo	Glicose monoidratada	16184808	6
Caelo	Glicose monoidratada	16184810	26
Caelo	Glicose monoidratada	16184816	3
Caelo	Glicose monoidratada	17005801	3
Caelo	Glicose monoidratada	17005802	12
Caelo	Glicose monoidratada	170058025312	1
Caelo	Glicose monoidratada	170058025458	1
Caelo	Glicose monoidratada	170058025517	1
Caelo	Glicose monoidratada	170058025621	1
Caelo	Glicose monoidratada	17005803	33
Caelo	Glicose monoidratada	17005804	10
Caelo	Glicose monoidratada	17005805	2
Caelo	Glicose monoidratada	17005811	2
Caelo	Glicose monoidratada	17005812	13
Caelo	Glicose monoidratada	17005813	7
Caelo	Glicose monoidratada	1701002-01	2
Caelo	Glicose monoidratada	170100401	1
Caelo	Glicose monoidratada	170323183	1
Caelo	Glicose monoidratada	1707004-001	1
Caelo	Glicose monoidratada	1707004-01	7
Caelo	Glicose monoidratada	17136801	31

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose monoidratada	17136801/P-11101722	1
Caelo	Glicose monoidratada	17136802	17
Caelo	Glicose monoidratada	17136804	20
Caelo	Glicose monoidratada	17136804x2	1
Caelo	Glicose monoidratada	17136805	14
Caelo	Glicose monoidratada	17305003	47
Caelo	Glicose monoidratada	17305004	13
Caelo	Glicose monoidratada	1801009	1
Caelo	Glicose monoidratada	1801009-01	4
Caelo	Glicose monoidratada	180101901	1
Caelo	Glicose monoidratada	180101907	1
Caelo	Glicose monoidratada	180300004	1
Caelo	Glicose monoidratada	18030003	15
Caelo	Glicose monoidratada	18030004	7
Caelo	Glicose monoidratada	18030005	7
Caelo	Glicose monoidratada	18030006	1
Caelo	Glicose monoidratada	1803006	1
Caelo	Glicose monoidratada	18064912	1
Caelo	Glicose monoidratada	180700501	1
Caelo	Glicose monoidratada	1807005-01	2
Caelo	Glicose monoidratada	1807005-02	1
Caelo	Glicose monoidratada	18071402	1
Caelo	Glicose monoidratada	18101901	67
Caelo	Glicose monoidratada	18101902	6
Caelo	Glicose monoidratada	18101903	24
Caelo	Glicose monoidratada	181019030	1
Caelo	Glicose monoidratada	18101907	34
Caelo	Glicose monoidratada	18101909	1
Caelo	Glicose monoidratada	18107907	1
Caelo	Glicose monoidratada	1810901	1
Caelo	Glicose monoidratada	1810907	1
Caelo	Glicose monoidratada	1811020-01	8
Caelo	Glicose monoidratada	181197	1
Caelo	Glicose monoidratada	181401903	1
Caelo	Glicose monoidratada	18214701	22
Caelo	Glicose monoidratada	18214702	1
Caelo	Glicose monoidratada	18214703	54
Caelo	Glicose monoidratada	18214704	20
Caelo	Glicose monoidratada	18214708	31
Caelo	Glicose monoidratada	18214709	5
Caelo	Glicose monoidratada	18214710	8
Caelo	Glicose monoidratada	18214712	1
Caelo	Glicose monoidratada	182414703	1
Caelo	Glicose monoidratada	1891009-01	1
Caelo	Glicose monoidratada	190073303	1
Caelo	Glicose monoidratada	190402901	1
Caelo	Glicose monoidratada	19073033	1
Caelo	Glicose monoidratada	19073301	12
Caelo	Glicose monoidratada	19073302	12
Caelo	Glicose monoidratada	190733023	1
Caelo	Glicose monoidratada	19073303	78
Caelo	Glicose monoidratada	19073304	18
Caelo	Glicose monoidratada	19073305	10
Caelo	Glicose monoidratada	19073309	29
Caelo	Glicose monoidratada	19073310	7
Caelo	Glicose monoidratada	190801201	2
Caelo	Glicose monoidratada	191486003	1
Caelo	Glicose monoidratada	19248600	1
Caelo	Glicose monoidratada	192486002	17
Caelo	Glicose monoidratada	192486003	68

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose monoidratada	192486004	25
Caelo	Glicose monoidratada	192486006	13
Caelo	Glicose monoidratada	192486007	9
Caelo	Glicose monoidratada	1973303	1
Caelo	Glicose monoidratada	200002144002	2
Caelo	Glicose monoidratada	2000214006	1
Caelo	Glicose monoidratada	20002144002	70
Caelo	Glicose monoidratada	20002144005	6
Caelo	Glicose monoidratada	20002144006	6
Caelo	Glicose monoidratada	20002144007	7
Caelo	Glicose monoidratada	20002144022	1
Caelo	Glicose monoidratada	200021444005	1
Caelo	Glicose monoidratada	20003963001	2
Caelo	Glicose monoidratada	20003964001	8
Caelo	Glicose monoidratada	20003964002	52
Caelo	Glicose monoidratada	20003964004	18
Caelo	Glicose monoidratada	20003964005	3
Caelo	Glicose monoidratada	20003964008	4
Caelo	Glicose monoidratada	20003964009	21
Caelo	Glicose monoidratada	20003964012	1
Caelo	Glicose monoidratada	20003964013	7
Caelo	Glicose monoidratada	20003964015	14
Caelo	Glicose monoidratada	20003964016	2
Caelo	Glicose monoidratada	20004180002	1
Caelo	Glicose monoidratada	2000418009	1
Caelo	Glicose monoidratada	200041820009	3
Caelo	Glicose monoidratada	20004182001	4
Caelo	Glicose monoidratada	20004182002	9
Caelo	Glicose monoidratada	20004182003	21
Caelo	Glicose monoidratada	20004182004	2
Caelo	Glicose monoidratada	20004182006	1
Caelo	Glicose monoidratada	20004182007	3
Caelo	Glicose monoidratada	20004182008	18
Caelo	Glicose monoidratada	20004182009	28
Caelo	Glicose monoidratada	20004182010	3
Caelo	Glicose monoidratada	2000418209	2
Caelo	Glicose monoidratada	2002144002	2
Caelo	Glicose monoidratada	2002144006	1
Caelo	Glicose monoidratada	200415PJK01	1
Caelo	Glicose monoidratada	2004182006	1
Caelo	Glicose monoidratada	2004182009	1
Caelo	Glicose monoidratada	2006007-01	2
Caelo	Glicose monoidratada	2009024-01	1
Caelo	Glicose monoidratada	2017Q-02209	1
Caelo	Glicose monoidratada	210018586004	1
Caelo	Glicose monoidratada	210018860008	3
Caelo	Glicose monoidratada	21001886003	10
Caelo	Glicose monoidratada	21001886004	25
Caelo	Glicose monoidratada	21001886005	19
Caelo	Glicose monoidratada	21001886008	5
Caelo	Glicose monoidratada	21001886009	9
Caelo	Glicose monoidratada	21001886011	6
Caelo	Glicose monoidratada	21001886013	2
Caelo	Glicose monoidratada	21002018013	1
Caelo	Glicose monoidratada	21004018003	6
Caelo	Glicose monoidratada	21004018006	5
Caelo	Glicose monoidratada	21004018007	16
Caelo	Glicose monoidratada	21004018009	6
Caelo	Glicose monoidratada	21004018011	1
Caelo	Glicose monoidratada	21004018013	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glicose monoidratada	21004018014	18
Caelo	Glicose monoidratada	21004018015	19
Caelo	Glicose monoidratada	21004018017	2
Caelo	Glicose monoidratada	21004018018	1
Caelo	Glicose monoidratada	2100886013	1
Caelo	Glicose monoidratada	2101402	1
Caelo	Glicose monoidratada	2103027-01	3
Caelo	Glicose monoidratada	2104018009	2
Caelo	Glicose monoidratada	219317005803	1
Caelo	Glicose monoidratada	22000456006	1
Caelo	Glicose monoidratada	22000756003	2
Caelo	Glicose monoidratada	22000756005	3
Caelo	Glicose monoidratada	22000756006	19
Caelo	Glicose monoidratada	22000756007	4
Caelo	Glicose monoidratada	22000756009	1
Caelo	Glicose monoidratada	22000756010	2
Caelo	Glicose monoidratada	22000756011	2
Caelo	Glicose monoidratada	22000756014	2
Caelo	Glicose monoidratada	22000756015	28
Caelo	Glicose monoidratada	22000756018	3
Caelo	Glicose monoidratada	22000756019	1
Caelo	Glicose monoidratada	22000756020	1
Caelo	Glicose monoidratada	22000756021	2
Caelo	Glicose monoidratada	22000756022	3
Caelo	Glicose monoidratada	220007567	1
Caelo	Glicose monoidratada	22001899002	3
Caelo	Glicose monoidratada	22001899003	1
Caelo	Glicose monoidratada	22001899005c	1
Caelo	Glicose monoidratada	220616(21004018009)	1
Caelo	Glicose monoidratada	220756015	1
Caelo	Glicose monoidratada	2222222222	1
Caelo	Glicose monoidratada	23000211004	3
Caelo	Glicose monoidratada	23000211008	1
Caelo	Glicose monoidratada	2300021104	1
Caelo	Glicose monoidratada	23051801	1
Caelo	Glicose monoidratada	2315Q-02209NP	1
Caelo	Glicose monoidratada	2316E-02209	1
Caelo	Glicose monoidratada	24081801	1
Caelo	Glicose monoidratada	26061802	1
Caelo	Glicose monoidratada	27081801	1
Caelo	Glicose monoidratada	2743	1
Caelo	Glicose monoidratada	2745	1
Caelo	Glicose monoidratada	2795	1
Caelo	Glicose monoidratada	28051507	1
Caelo	Glicose monoidratada	3612J-02209	1
Caelo	Glicose monoidratada	4616M-02209	1
Caelo	Glicose monoidratada	5051401	1
Caelo	Glicose monoidratada	5092	1
Caelo	Glicose monoidratada	613011-3p	1
Caelo	Glicose monoidratada	716I-02209	1
Caelo	Glicose monoidratada	718A-02209	1
Caelo	Glicose monoidratada	719092G	1
Caelo	Glicose monoidratada	72714068	1
Caelo	Glicose monoidratada	8697	1
Caelo	Glicose monoidratada	E144C	1
Caelo	Glicose monoidratada	E388S	1
Caelo	Glicose monoidratada	Test	1
Caelo	Glicose monoidratada	UIUJHJH	1
Caeo	Glicose monoidratada	1049103	1
Caeolo / noweda	Glicose monoidratada		1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caeolo/Noweda	Glicose monoidratada	15413301	1
Caeolo/Phönix	Glicose monoidratada	16184810	2
Caesa/Phoenix	Glicose monoidratada	15413304	1
Caesar & Lorenz	Glicose monoidratada	13157007	1
Caesar & Loretz / Gehe	Glicose monoidratada	18214703	3
Caesar & Loretz GmbH…	Glicose monoidratada	19073305	1
Caesar & Loretz GmbH…	Glicose monoidratada	19073310	3
Caesar & Loretz GmbH…	Glicose monoidratada	19073303	2
Caesar & Loretz GmbH…	Glicose monoidratada	19073309	2
Caesar & Loretz GmbH…	Glicose monoidratada	192486003	3
Caesar & Loretz GmbH…	Glicose monoidratada	20003964002	1
Caesar & Loretz GmbH…	Glicose monoidratada	192486006	2
Caesar & Loretz GmbH…	Glicose monoidratada	20003964001	1
Caesar & Loretz GmbH…	Glicose monoidratada	20004182001	1
Caesar & Loretz GmbH…	Glicose monoidratada	21001886008	2
Caesar & Loretz GmbH…	Glicose monoidratada	21004018006	1
Caesar & Loretz GmbH…	Glicose monoidratada	21004018016	4
Caesar & Loretz GmbH…	Glicose monoidratada	21004018017	1
Caesar & Loretz GmbH…	Glicose monoidratada	22000756012	1
Caesar & Loretz GmbH…	Glicose monoidratada	192486007	3
Caesar & Loretz GmbH…	Glicose monoidratada	20003964008	1
Caesar & Loretz GmbH…	Glicose monoidratada	20004182006	1
Caesar & Loretz GmbH…	Glicose monoidratada	21001886003	1
Caesar & Loretz GmbH…	Glicose monoidratada	18214703	3
Caesar & Loretz GmbH L 50	Glicose monoidratada	22000756006	2
Caesar & Loretz GmbH…	Glicose monoidratada	21001886008	1
Caesar & Loretz GmbH…	Glicose monoidratada	20003964009	2
Caesar & Loretz GmbH…	Glicose monoidratada	21004018009	1
Caesar & Loretz GmbH/AEP	Glicose monoidratada	18214703	1
Caesar & Loretz GmbH/AEP	Glicose monoidratada	192486004	6
Caesar & Loretz GmbH/AHD	Glicose monoidratada	22000756004	1
Caesar & Loretz GmbH/AHD	Glicose monoidratada	22000756022	1
Caesar & Loretz GmbH…	Glicose monoidratada	192486002	2
Caesar & Loretz GmbH…	Glicose monoidratada	19073310	1
Caesar & Loretz GmbH…	Glicose monoidratada	192486007	1
Caesar & Loretz GmbH…	Glicose monoidratada	192486003	3
Caesar & Loretz GmbH…	Glicose monoidratada	20002144002	1
Caesar & Loretz GmbH/G	Glicose monoidratada	20003964002	1
Caesar & Loretz GmbH/Gehe	Glicose monoidratada	192486003	1
Caesar & Loretz GmbH/Gehe	Glicose monoidratada	20002144002	1
Caesar & Loretz GmbH/Gehe	Glicose monoidratada	20004182008	1
Caesar & Loretz GmbH/Gehe	Glicose monoidratada	21004018006	1
Caesar & Loretz GmbH…	Glicose monoidratada	20002144005	1
Caesar & Loretz GmbH/Gö	Glicose monoidratada	20002144002	1
Caesar & Loretz GmbH…	Glicose monoidratada	20002144002	1
Caesar & Loretz GmbH…	Glicose monoidratada	2009024-01	1
Caesar & Loretz GmbH/K	Glicose monoidratada	21004018014	1
Caesar & Loretz GmbH/Kehr	Glicose monoidratada	18214704	1
Caesar & Loretz GmbH…	Glicose monoidratada	20002144002	4
Caesar & Loretz GmbH…	Glicose monoidratada	20003964015	1
Caesar & Loretz GmbH…	Glicose monoidratada	20004182009	4
Caesar & Loretz GmbH/L10	Glicose monoidratada	21004018015	1
Caesar & Loretz GmbH…	Glicose monoidratada	19073303	3
Caesar & Loretz GmbH…	Glicose monoidratada	20004182008	2
Caesar & Loretz GmbH…	Glicose monoidratada	20004182003	2
Caesar & Loretz GmbH…	Glicose monoidratada	20004182006	1
Caesar & Loretz GmbH…	Glicose monoidratada	21001886008	1
Caesar & Loretz GmbH…	Glicose monoidratada	21004018009	2
Caesar & Loretz GmbH…	Glicose monoidratada	22001899001	1
Caesar & Loretz GmbH…	Glicose monoidratada	19073303	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Glicose monoidratada	19073309	4
Caesar & Loretz GmbH...	Glicose monoidratada	20003964002	5
Caesar & Loretz GmbH...	Glicose monoidratada	20003964009	3
Caesar & Loretz GmbH...	Glicose monoidratada	20004182009	2
Caesar & Loretz GmbH...	Glicose monoidratada	21004018007	1
Caesar & Loretz GmbH...	Glicose monoidratada	21004018015	1
Caesar & Loretz GmbH...	Glicose monoidratada	22000756006	1
Caesar & Loretz GmbH...	Glicose monoidratada	22000756006	2
Caesar & Loretz GmbH...	Glicose monoidratada	22000756015	2
Caesar & Loretz GmbH...	Glicose monoidratada	22001899005	2
Caesar & Loretz GmbH...	Glicose monoidratada	20002144002	1
Caesar & Loretz GmbH...	Glicose monoidratada	20003964002	1
Caesar & Loretz GmbH...	Glicose monoidratada	20003964004	1
Caesar & Loretz GmbH...	Glicose monoidratada	20004182003	1
Caesar & Loretz GmbH...	Glicose monoidratada	21001886004	1
Caesar & Loretz GmbH	Glicose monoidratada	128214703	1
Caesar & Loretz GmbH	Glicose monoidratada	15180010	1
Caesar & Loretz GmbH	Glicose monoidratada	15180013	1
Caesar & Loretz GmbH	Glicose monoidratada	15413402	1
Caesar & Loretz GmbH	Glicose monoidratada	17005802	1
Caesar & Loretz GmbH	Glicose monoidratada	18101901	1
Caesar & Loretz GmbH	Glicose monoidratada	18101907	3
Caesar & Loretz GmbH	Glicose monoidratada	18179716	1
Caesar & Loretz GmbH	Glicose monoidratada	18214701	1
Caesar & Loretz GmbH	Glicose monoidratada	18214703	19
Caesar & Loretz GmbH	Glicose monoidratada	18214704	2
Caesar & Loretz GmbH	Glicose monoidratada	18214708	5
Caesar & Loretz GmbH	Glicose monoidratada	18214710	1
Caesar & Loretz GmbH	Glicose monoidratada	19073301	1
Caesar & Loretz GmbH	Glicose monoidratada	19073302	3
Caesar & Loretz GmbH	Glicose monoidratada	19073303	24
Caesar & Loretz GmbH	Glicose monoidratada	19073304	10
Caesar & Loretz GmbH	Glicose monoidratada	19073305	1
Caesar & Loretz GmbH	Glicose monoidratada	19073309	8
Caesar & Loretz GmbH	Glicose monoidratada	19073310	5
Caesar & Loretz GmbH	Glicose monoidratada	192486002	5
Caesar & Loretz GmbH	Glicose monoidratada	192486003	16
Caesar & Loretz GmbH	Glicose monoidratada	192486004	4
Caesar & Loretz GmbH	Glicose monoidratada	192486006	3
Caesar & Loretz GmbH	Glicose monoidratada	192486007	1
Caesar & Loretz GmbH	Glicose monoidratada	20000461007	1
Caesar & Loretz GmbH	Glicose monoidratada	20002144002	7
CAESAR & LORETZ GMBH	Glicose monoidratada	20002144002	4
Caesar & Loretz GmbH	Glicose monoidratada	20002144005	1
Caesar & Loretz GmbH	Glicose monoidratada	20002144006	7
Caesar & Loretz GmbH	Glicose monoidratada	20002144007	2
Caesar & Loretz GmbH	Glicose monoidratada	20003963001	4
Caesar & Loretz GmbH	Glicose monoidratada	20003964001	2
Caesar & Loretz GmbH	Glicose monoidratada	20003964002	18
Caesar & Loretz GmbH	Glicose monoidratada	20003964004	3
Caesar & Loretz GmbH	Glicose monoidratada	20003964005	4
Caesar & Loretz GmbH	Glicose monoidratada	20003964008	1
Caesar & Loretz GmbH	Glicose monoidratada	20003964009	9
Caesar & Loretz GmbH	Glicose monoidratada	20003964012	6
Caesar & Loretz GmbH	Glicose monoidratada	20003964013	1
Caesar & Loretz GmbH	Glicose monoidratada	20003964015	4
Caesar & Loretz GmbH	Glicose monoidratada	20003964016	4
Caesar & Loretz GmbH	Glicose monoidratada	20004182001	2
Caesar & Loretz GmbH	Glicose monoidratada	20004182002	11
Caesar & Loretz GmbH	Glicose monoidratada	20004182003	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Glicose monoidratada	20004182004	1
Caesar & Loretz GmbH	Glicose monoidratada	20004182006	2
Caesar & Loretz GmbH	Glicose monoidratada	20004182007	2
Caesar & Loretz GmbH	Glicose monoidratada	20004182008	9
Caesar & Loretz GmbH	Glicose monoidratada	20004182009	16
Caesar & Loretz GmbH	Glicose monoidratada	20004182010	1
Caesar & Loretz GmbH	Glicose monoidratada	2004182010	1
Caesar & Loretz GmbH	Glicose monoidratada	21001886003	1
Caesar & Loretz GmbH	Glicose monoidratada	21001886004	5
Caesar & Loretz GmbH	Glicose monoidratada	21001886005	16
CAESAR & LORETZ GMBH	Glicose monoidratada	21001886005	3
Caesar & Loretz GmbH	Glicose monoidratada	21001886008	3
Caesar & Loretz GmbH	Glicose monoidratada	21001886009	5
Caesar & Loretz GmbH	Glicose monoidratada	21001886011	3
Caesar & Loretz GmbH	Glicose monoidratada	21004018003	2
Caesar & Loretz GmbH	Glicose monoidratada	21004018006	3
Caesar & Loretz GmbH	Glicose monoidratada	21004018007	6
Caesar & Loretz GmbH	Glicose monoidratada	21004018009	2
Caesar & Loretz GmbH	Glicose monoidratada	21004018011	1
Caesar & Loretz GmbH	Glicose monoidratada	21004018013	1
Caesar & Loretz GmbH	Glicose monoidratada	21004018014	10
Caesar & Loretz GmbH	Glicose monoidratada	21004018015	9
Caesar & Loretz GmbH	Glicose monoidratada	2102027-1	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756004	2
Caesar & Loretz GmbH	Glicose monoidratada	22000756006	5
Caesar & Loretz GmbH	Glicose monoidratada	22000756007	4
Caesar & Loretz GmbH	Glicose monoidratada	22000756009	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756010	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756011	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756012	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756013	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756014	2
Caesar & Loretz GmbH	Glicose monoidratada	22000756015	21
Caesar & Loretz GmbH	Glicose monoidratada	22000756017	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756018	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756020	2
Caesar & Loretz GmbH	Glicose monoidratada	22000756021	1
Caesar & Loretz GmbH	Glicose monoidratada	22000756022	4
Caesar & Loretz GmbH	Glicose monoidratada	22001899001	3
Caesar & Loretz GmbH	Glicose monoidratada	22001899002	4
Caesar & Loretz GmbH	Glicose monoidratada	22001899010	1
Caesar & Loretz GmbH	Glicose monoidratada	22001899012	2
Caesar & Loretz GmbH	Glicose monoidratada	23000211001	1
Caesar & Loretz GmbHKehr	Glicose monoidratada	192486002	1
Caesar & Loretz/ Cae...	Glicose monoidratada	18030004	1
Caesar & Loretz/Noweda	Glicose monoidratada	16049102	1
Caesar & Loretz/Phönix	Glicose monoidratada	18101907	1
Caesar & Loretz	Glicose monoidratada	21001886008	1
Caesar & Loretz	Glicose monoidratada	22000756004	1
Caesar & Loretz	Glicose monoidratada	22000756010	1
Caesar / Gehe	Glicose monoidratada	17005802	1
Caesar und Loretz GmbH	Glicose monoidratada	16184807	1
Caesar&Loretz GmbH	Glicose monoidratada	22000756005	1
Caesar&Loretz GmbH	Glicose monoidratada	22000756009	1
Calo	Glicose monoidratada	15180010	2
Cealo/ Noweda	Glicose monoidratada	15413412	1
Cealo/Noweda	Glicose monoidratada	20003964012	2
Cealo/Sanacorp	Glicose monoidratada	22000756015	1
Cealo	Glicose monoidratada	13157017	1
Cealo	Glicose monoidratada	14102430	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Celo/Jenne	Glicose monoidratada	20003964009	1
Dermapharm	Glicose monoidratada	1601016-02	1
dextro energy / Noweda	Glicose monoidratada	L1299	1
Dextro Energy GmbH/Gehe	Glicose monoidratada	L4163	2
Dextro Energy GmbH/Gehe	Glicose monoidratada	L4164	1
Dextro Energy GmbH/Gehe	Glicose monoidratada	L4274	1
Dextro Energy GmbH/S...	Glicose monoidratada	L1299	1
Dextro Energy GmbH	Glicose monoidratada	5/2018L6315	1
Dextro energy/ Fiebig	Glicose monoidratada	L1147	1
Dextro Energy/Gehe	Glicose monoidratada	L1147	1
Dextro energy	Glicose monoidratada	L0086	1
Dextro energy	Glicose monoidratada	L0097	1
Dextro Energy	Glicose monoidratada	13171	1
dextro energy	Glicose monoidratada	19016127	1
dextro energy	Glicose monoidratada	19050634	1
Dextro EnergyGmbH	Glicose monoidratada	L4036	1
Dextro EnergyGmbH	Glicose monoidratada	L4273	1
Dextro ernergy Gmbh	Glicose monoidratada	L6043	1
Dextro GmbH/Noweda	Glicose monoidratada	L5301	1
Dextro/Krieger/15.05.13	Glicose monoidratada	13092	1
DextroEnergy/Noweda	Glicose monoidratada	L2283	1
dextroenergy	Glicose monoidratada	190161027	1
Dr. Aug. Wolff GmbH ...	Glicose monoidratada	21001886011	1
Eigenherstellung	Glicose monoidratada	110912HML01	1
Eigenherstellung	Glicose monoidratada	110913HJK02	1
Eigenherstellung	Glicose monoidratada	120912HML02	1
Eigenherstellung	Glicose monoidratada	160915HML01	1
Eigenherstellung	Glicose monoidratada	180213HJK01	1
Eigenherstellung	Glicose monoidratada	30912HML01	1
Eigenherstellung	Glicose monoidratada	40615HJK01	1
Eurho / Alliance	Glicose monoidratada	2001006-01	2
EuRho / Alliance	Glicose monoidratada	2103027-01	1
EuRho Noweda	Glicose monoidratada	2006007-01	1
EuRho/ Kehr	Glicose monoidratada	220201501	1
EuRho/Gehe 09.07.2022	Glicose monoidratada	2202015-01	1
EuRho/GEHE	Glicose monoidratada	1410019-01	1
EuRho/GEHE	Glicose monoidratada	1904029-01	2
EuRho/Noweda	Glicose monoidratada	2103027-01	7
EuRho/Phoenix	Glicose monoidratada	140500401	1
EuRho/Phoenix	Glicose monoidratada	1604006-01	1
EuRho/Phoenix	Glicose monoidratada	221005-02	1
Eurho/Sanacorp	Glicose monoidratada	1108061-01	2
EuRho	Glicose monoidratada	1108061-01	2
EuRho	Glicose monoidratada	1108061-02	1
EuRho	Glicose monoidratada	1204044-01	2
EuRho	Glicose monoidratada	151780	1
EuRho	Glicose monoidratada	1604006-0104932048	1
EuRho	Glicose monoidratada	1707004-01	2
EuRho	Glicose monoidratada	2006007-01	1
EuRho	Glicose monoidratada	2103027-01	1
EuRho	Glicose monoidratada	2710Q-02209	1
Euro OT>C	Glicose monoidratada	2006007-01	2
Euro OTC	Glicose monoidratada		1
Euro OTC	Glicose monoidratada	103027-012	3
Euro OTC	Glicose monoidratada	1103027-01	1
Euro OTC	Glicose monoidratada	1108061-01	2
Euro OTC	Glicose monoidratada	1114U2209	1
Euro OTC	Glicose monoidratada	1204044-01	1
Euro OTC	Glicose monoidratada	1204044-02	3
Euro OTC	Glicose monoidratada	1210034-01	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Glicose monoidratada	1210034-02	10
Euro OTC	Glicose monoidratada	1210034-03	1
Euro OTC	Glicose monoidratada	130503001	1
Euro OTC	Glicose monoidratada	1305030-01	6
Euro OTC	Glicose monoidratada	1305030-02	6
Euro OTC	Glicose monoidratada	1305030-02	1
Euro OTC	Glicose monoidratada	140004-01	1
Euro OTC	Glicose monoidratada	14005004-02	1
Euro OTC	Glicose monoidratada	140101901	1
Euro OTC	Glicose monoidratada	1401019-01	15
Euro OTC	Glicose monoidratada	140101902	2
Euro OTC	Glicose monoidratada	140500401	1
Euro OTC	Glicose monoidratada	1405004-01	16
Euro OTC	Glicose monoidratada	140500402	1
Euro OTC	Glicose monoidratada	1405004-02	4
Euro OTC	Glicose monoidratada	1406212209	1
Euro OTC	Glicose monoidratada	141001901	1
Euro OTC	Glicose monoidratada	1410019-01	7
Euro OTC	Glicose monoidratada	1410019-02	4
Euro OTC	Glicose monoidratada	150402801	1
Euro OTC	Glicose monoidratada	1504028-01	14
Euro OTC	Glicose monoidratada	1504028-02	10
Euro OTC	Glicose monoidratada	15040281	1
Euro OTC	Glicose monoidratada	150900601	1
Euro OTC	Glicose monoidratada	1509006-01	19
Euro OTC	Glicose monoidratada	1509006-02	5
Euro OTC	Glicose monoidratada	1509006-1	1
Euro OTC	Glicose monoidratada	15095601	1
Euro OTC	Glicose monoidratada	151780	1
Euro OTC	Glicose monoidratada	15180010	1
Euro OTC	Glicose monoidratada	160101601	2
Euro OTC	Glicose monoidratada	1601016-01	23
Euro OTC	Glicose monoidratada	1601016-02	5
Euro OTC	Glicose monoidratada	16040060-01	1
Euro OTC	Glicose monoidratada	1604006-01	33
Euro OTC	Glicose monoidratada	160400602	2
Euro OTC	Glicose monoidratada	1604006-02	30
Euro OTC	Glicose monoidratada	1607024	1
Euro OTC	Glicose monoidratada	1607024-01	19
Euro OTC	Glicose monoidratada	1607024-02	31
Euro OTC	Glicose monoidratada	160704-01	1
Euro OTC	Glicose monoidratada	16184807	1
Euro OTC	Glicose monoidratada	1701002_01	1
Euro OTC	Glicose monoidratada	1701002-01	29
Euro OTC	Glicose monoidratada	170100202	1
Euro OTC	Glicose monoidratada	1701002-02	7
Euro OTC	Glicose monoidratada	1707004	1
Euro OTC	Glicose monoidratada	1707004-001	1
Euro OTC	Glicose monoidratada	170700401	2
Euro OTC	Glicose monoidratada	1707004-01	69
Euro OTC	Glicose monoidratada	170704401	1
Euro OTC	Glicose monoidratada	17136801	1
Euro OTC	Glicose monoidratada	17136804	1
Euro OTC	Glicose monoidratada	180100-01	1
Euro OTC	Glicose monoidratada	1801009_01	1
Euro OTC	Glicose monoidratada	180100901	2
Euro OTC	Glicose monoidratada	1801009-01	75
Euro OTC	Glicose monoidratada	180100941	1
Euro OTC	Glicose monoidratada	18070005-001	1
Euro OTC	Glicose monoidratada	180700501	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Glicose monoidratada	1807005-01	45
Euro OTC	Glicose monoidratada	1807005-02	4
Euro OTC	Glicose monoidratada	18070501	1
Euro OTC	Glicose monoidratada	18070521	1
Euro OTC	Glicose monoidratada	18101901	2
Euro OTC	Glicose monoidratada	18101907	1
Euro OTC	Glicose monoidratada	181101001	1
Euro OTC	Glicose monoidratada	1811020	1
Euro OTC	Glicose monoidratada	181102001	2
Euro OTC	Glicose monoidratada	1811020-01	37
Euro OTC	Glicose monoidratada	1811020-02	8
Euro OTC	Glicose monoidratada	181102003	1
Euro OTC	Glicose monoidratada	1811020-1	1
Euro OTC	Glicose monoidratada	18110201-02	1
Euro OTC	Glicose monoidratada	18111020-01	1
Euro OTC	Glicose monoidratada	18214704	1
Euro OTC	Glicose monoidratada	187005-001	1
Euro OTC	Glicose monoidratada	1900402901	1
Euro OTC	Glicose monoidratada	1904029	1
Euro OTC	Glicose monoidratada	1904029/01	1
Euro OTC	Glicose monoidratada	190402901	4
Euro OTC	Glicose monoidratada	1904029-01	53
Euro OTC	Glicose monoidratada	190429-01	1
Euro OTC	Glicose monoidratada	1907012-01	1
Euro OTC	Glicose monoidratada	1908010-01	1
Euro OTC	Glicose monoidratada	1908012-01	56
Euro OTC	Glicose monoidratada	19080122-01	1
Euro OTC	Glicose monoidratada	190801241	1
Euro OTC	Glicose monoidratada	200007-01	1
Euro OTC	Glicose monoidratada	20009024-01	1
Euro OTC	Glicose monoidratada	2001006-001	1
Euro OTC	Glicose monoidratada	200100601	6
Euro OTC	Glicose monoidratada	2001006-01	67
Euro OTC	Glicose monoidratada	200600-01	1
Euro OTC	Glicose monoidratada	200600701	4
Euro OTC	Glicose monoidratada	2006007-01	48
Euro OTC	Glicose monoidratada	200902401	3
Euro OTC	Glicose monoidratada	2009024-01	105
Euro OTC	Glicose monoidratada	200902-41	1
Euro OTC	Glicose monoidratada	2013U-02209	1
Euro OTC	Glicose monoidratada	20160405-04	1
Euro OTC	Glicose monoidratada	2023012-1	1
Euro OTC	Glicose monoidratada	2103027	4
Euro OTC	Glicose monoidratada	210302701	2
Euro OTC	Glicose monoidratada	2103027-01	102
Euro OTC	Glicose monoidratada	210307-01	1
Euro OTC	Glicose monoidratada	2103207-01	1
Euro OTC	Glicose monoidratada	210327	1
Euro OTC	Glicose monoidratada	2107024_02	2
Euro OTC	Glicose monoidratada	2107024-01	29
Euro OTC	Glicose monoidratada	2107024-02	50
Euro OTC	Glicose monoidratada	2107042-02	1
Euro OTC	Glicose monoidratada	210724-02	1
Euro OTC	Glicose monoidratada	2109008	1
Euro OTC	Glicose monoidratada	2109008-01	33
Euro OTC	Glicose monoidratada	2109008-02	13
Euro OTC	Glicose monoidratada	219008-01	1
Euro OTC	Glicose monoidratada	2202015/01	1
Euro OTC	Glicose monoidratada	2202015-01	27
Euro OTC	Glicose monoidratada	2202015-02	30

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Glicose monoidratada	2202015-03	4
Euro OTC	Glicose monoidratada	22022015-01	1
Euro OTC	Glicose monoidratada	220601801	1
Euro OTC	Glicose monoidratada	2206018-01	46
Euro OTC	Glicose monoidratada	2206018-02	5
Euro OTC	Glicose monoidratada	2210005-01	5
Euro OTC	Glicose monoidratada	2210005-02	13
Euro OTC	Glicose monoidratada	226018-01	1
Euro OTC	Glicose monoidratada	2302007-01	3
Euro OTC	Glicose monoidratada	23051802	1
Euro OTC	Glicose monoidratada	2313E-02209	1
Euro OTC	Glicose monoidratada	31102013B	1
Euro OTC	Glicose monoidratada	8638943	1
Euro OTC	Glicose monoidratada	96-01	1
Euro OTC	Glicose monoidratada	E024R	1
Euro OTC	Glicose monoidratada	E042R/2009024-01	1
Euro OTC	Glicose monoidratada	E108T	3
Euro OTC	Glicose monoidratada	E255L	1
Euro OTC	Glicose monoidratada	E267X	1
Euro OTC	Glicose monoidratada	E388S	2
Euro OTC	Glicose monoidratada	E470S	2
Euro OTC	Glicose monoidratada	E617K	1
Euro OTC	Glicose monoidratada	E643N	1
Euro OTC	Glicose monoidratada	E732N	2
Euro OTC	Glicose monoidratada	E777P	2
Euro OTC	Glicose monoidratada	E882R	1
Euro OTC	Glicose monoidratada	E961M	1
Euro OTG/ AHD	Glicose monoidratada	1701002-01	1
Euro OTG/ AHD	Glicose monoidratada	1801009-01	1
Euro Pharma/Phönix	Glicose monoidratada	2103027-01	3
EuRo/ Noweda	Glicose monoidratada	1904029-01	1
Euro/ Sanacorp	Glicose monoidratada	1504028-01	1
Euro/Alliance Healthcare	Glicose monoidratada	1604006-01	1
Euro/Krieger	Glicose monoidratada	1807005-01	1
Euro/Noweda	Glicose monoidratada	1604006-02	2
Euro/Phoenix	Glicose monoidratada	210724-01	1
Euro/Phönix	Glicose monoidratada	1707004-01	1
Euro/Phönix	Glicose monoidratada	1811020-01	1
Euro/Phönix	Glicose monoidratada	1811020-02	1
Euro/Phönix	Glicose monoidratada	2210005-01	1
Euroo	Glicose monoidratada	1604006-01	1
Fagron	Glicose monoidratada		1
Fagron	Glicose monoidratada	11L19-N13	1
Fagron	Glicose monoidratada	12B09-N05	1
Fagron	Glicose monoidratada	12G30-N01	12
Fagron	Glicose monoidratada	12G30-NO1	2
Fagron	Glicose monoidratada	13A_N01	1
Fagron	Glicose monoidratada	13A25-n01	1
Fagron	Glicose monoidratada	13A25-N01	6
Fagron	Glicose monoidratada	13A25-No1	1
Fagron	Glicose monoidratada	13A25-NO1	2
Fagron	Glicose monoidratada	13B01-N03	5
Fagron	Glicose monoidratada	13C25N09	2
Fagron	Glicose monoidratada	13C25-N09	8
Fagron	Glicose monoidratada	13h06-n08	1
Fagron	Glicose monoidratada	13H06-N08	17
Fagron	Glicose monoidratada	13H14-B06-289483	1
Fagron	Glicose monoidratada	1401019-01	1
Fagron	Glicose monoidratada	1404-B08-298601	2
Fagron	Glicose monoidratada	1404-B08-298604	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Glicose monoidratada	1407-808-307707	1
Fagron	Glicose monoidratada	14102420	1
Fagron	Glicose monoidratada	14104-B08-302707	1
Fagron	Glicose monoidratada	14B04-B01	3
Fagron	Glicose monoidratada	14B04-B01-291137	7
Fagron	Glicose monoidratada	14B04-B01-291138	3
Fagron	Glicose monoidratada	14B04-B01-291143	2
Fagron	Glicose monoidratada	14B28-B02	2
Fagron	Glicose monoidratada	14b28-b02-291353	1
Fagron	Glicose monoidratada	14B28-B02-291353	11
Fagron	Glicose monoidratada	14B28-B02-291354	3
Fagron	Glicose monoidratada	14D30-B06-294678	1
Fagron	Glicose monoidratada	14D30-bo6-294678	1
Fagron	Glicose monoidratada	14I04-808	1
Fagron	Glicose monoidratada	14I04-B08	1
Fagron	Glicose monoidratada	14I04-B08-298601	1
Fagron	Glicose monoidratada	14I04-B08-298602	3
Fagron	Glicose monoidratada	14I04B8298602	1
Fagron	Glicose monoidratada	1509006-01	1
Fagron	Glicose monoidratada	151780-0004	1
Fagron	Glicose monoidratada	1521-B06-309508	1
Fagron	Glicose monoidratada	15A21-B06-309508	3
Fagron	Glicose monoidratada	15B01291137	1
Fagron	Glicose monoidratada	17136805	1
Fagron	Glicose monoidratada	18101903	2
Fagron	Glicose monoidratada	270313PML01	1
Fagron	Glicose monoidratada	3413E-02209	1
Fagron	Glicose monoidratada	4213Q-02209	1
Fagron	Glicose monoidratada	4562135	1
Fagron	Glicose monoidratada	8G31-N09	1
Fagron	Glicose monoidratada	E0AJ5	1
Fagron	Glicose monoidratada	E144C	1
Fagron	Glicose monoidratada	E524W	1
Fagron	Glicose monoidratada	E571X	1
Fargon	Glicose monoidratada	13C25-N09	1
Fargron	Glicose monoidratada	13A25-N01	1
Fiebig/ Dextropur	Glicose monoidratada	L7045	1
Fiebig	Glicose monoidratada	18101907	1
Fragon	Glicose monoidratada	13H06-N08	1
Frey+Lau GmbH	Glicose monoidratada	1601016-01	1
GATT-KOLLER/PHOENIX	Glicose monoidratada	243/02141714	1
GATT-KOLLER/PHOENIX	Glicose monoidratada	243/02142614	1
Gehe	Glicose monoidratada	13157026	2
GEHE	Glicose monoidratada	17005803	1
Gehe	Glicose monoidratada	1707004-01	1
GEHE	Glicose monoidratada	1707004-01	1
Gehe	Glicose monoidratada	17305003	1
GEHE	Glicose monoidratada	18030003	2
Gehe	Glicose monoidratada	18101907	1
Gehe	Glicose monoidratada	18214703	1
Gehe	Glicose monoidratada	22001899011	4
Gehe	Glicose monoidratada	23000211001	1
Gehe	Glicose monoidratada	2302007-01	6
geibo	Glicose monoidratada	220601801	1
Gutenberg-Apotheke	Glicose monoidratada	14B04-B01	1
hzdjfdj	Glicose monoidratada	jdhdfhhf	1
Jenne	Glicose monoidratada	2009024-01	1
Jenne	Glicose monoidratada	22001899002	1
Jenne	Glicose monoidratada	2210005-02	2
Kehr	Glicose monoidratada	18101907	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Glicose monoidratada	22000756019	1
Kehr	Glicose monoidratada	23000211010	1
Klenk	Glicose monoidratada	112233	1
Klosterring	Glicose monoidratada	17136802	1
Kyberg Experts	Glicose monoidratada	L9009	1
Mohrenapo	Glicose monoidratada	192486003	1
Noweda 10.02.2015	Glicose monoidratada	14334802	3
Noweda 10.032016	Glicose monoidratada	15413304	2
Noweda 30.07.2015	Glicose monoidratada	15095612	1
Noweda/apo-ident	Glicose monoidratada	210702402	1
Noweda/EuRho 01.02.2...	Glicose monoidratada	2009024-01	1
Noweda	Glicose monoidratada	1204044-01	2
Noweda	Glicose monoidratada	1210034	1
Noweda	Glicose monoidratada	151780	1
Noweda	Glicose monoidratada	1601016-01	1
Noweda	Glicose monoidratada	1607024-02	1
Noweda	Glicose monoidratada	17005801	1
Noweda	Glicose monoidratada	1701002-01	2
Noweda	Glicose monoidratada	1807005-01	1
Noweda	Glicose monoidratada	18101909	1
Noweda	Glicose monoidratada	1811020-02	1
Noweda	Glicose monoidratada	1904029-01	3
Noweda	Glicose monoidratada	1908012-01	2
Noweda	Glicose monoidratada	2006007-01E777P	1
Noweda	Glicose monoidratada	200902401	2
Noweda	Glicose monoidratada	2009024-01	1
Noweda	Glicose monoidratada	2107024-02	1
Noweda	Glicose monoidratada	22000756006	2
Noweda	Glicose monoidratada	22001899010	1
NOWEDA	Glicose monoidratada	2206018-01	1
Noweda	Glicose monoidratada	2210005-02	1
Noweda	Glicose monoidratada	2230756007	1
Noweda	Glicose monoidratada	A000018	1
Noweda	Glicose monoidratada	E882R	2
Pala	Glicose monoidratada	18214704	1
Pala	Glicose monoidratada	192486002	1
Ph.Eur.8.0	Glicose monoidratada	1401019-02	1
ph.Eur	Glicose monoidratada	2206018-01	1
pharma gmbh	Glicose monoidratada	1401019-01	1
Phoenix/Cealo	Glicose monoidratada	17305004	1
Phoenix	Glicose monoidratada	1707004-01	1
Phoenix	Glicose monoidratada	18101901	1
Phoenix	Glicose monoidratada	18214710	1
Phoenix	Glicose monoidratada	192486002	1
Phoenix	Glicose monoidratada	192486007	1
Phoenix	Glicose monoidratada	20003963001	1
Phoenix	Glicose monoidratada	2100186003	1
Phoenix	Glicose monoidratada	210702402	1
Phoenix	Glicose monoidratada	210800_01	1
Phoenix	Glicose monoidratada	22000756006	1
Phoenix	Glicose monoidratada	22000756019	1
Phoenix	Glicose monoidratada	2302007-01	2
Phoenix	Glicose monoidratada	3242	1
Phoenix	Glicose monoidratada	3385	1
Phönix Gotha	Glicose monoidratada	1401019-01	1
Phönix Gotha	Glicose monoidratada	1405004-02	1
Phönix Gotha	Glicose monoidratada	17136801	1
Phönix Gotha	Glicose monoidratada	17305003	1
Phönix Gotha	Glicose monoidratada	18101901	1
Phönix Gotha	Glicose monoidratada	18214703	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix Gotha	Glicose monoidratada	19073303	2
Phönix Gotha	Glicose monoidratada	192486003	1
Phönix	Glicose monoidratada	1210334-02	1
Phönix	Glicose monoidratada	1401019-01	1
phönix	Glicose monoidratada	16049101	1
phönix	Glicose monoidratada	16049104	1
phönix	Glicose monoidratada	16184816	1
Phönix	Glicose monoidratada	1801009-01	1
Phönix	Glicose monoidratada	18030005	1
Phönix	Glicose monoidratada	1807005-01	1
Phönix	Glicose monoidratada	18101901	2
Phönix	Glicose monoidratada	18101907	1
Phönix	Glicose monoidratada	18214703	1
Phönix	Glicose monoidratada	1904029-01	1
Phönix	Glicose monoidratada	19073304	1
Phönix	Glicose monoidratada	192486003	1
Phönix	Glicose monoidratada	200002144002	1
Phönix	Glicose monoidratada	20003963001	1
Phönix	Glicose monoidratada	20003964009	1
Phönix	Glicose monoidratada	20004182009	1
Phönix	Glicose monoidratada	200100601	1
Phönix	Glicose monoidratada	2006007-01	1
Phönix	Glicose monoidratada	21004018014	1
Phönix	Glicose monoidratada	22001899010	1
phönix	Glicose monoidratada	2202015-03	1
phönix	Glicose monoidratada	2206018-01	1
Phönix	Glicose monoidratada	23000211006	3
Phönix	Glicose monoidratada	23003430001	1
Roquette Freres/AHD	Glicose monoidratada	12G30-N01	1
Roquette Lestrem FR/…	Glicose monoidratada	1210034-02	1
Roquette Lestrem	Glicose monoidratada	160702402	1
Roquette Lestrem	Glicose monoidratada	1904029-01	8
roquette lestrem	Glicose monoidratada	2009024-01	2
Roquette/Phoenix	Glicose monoidratada	E732N	1
sana	Glicose monoidratada	15095601	2
Sanacop	Glicose monoidratada		1
Sanacorp,30.03.17, 7,12EUR	Glicose monoidratada	16184810	1
Sanacorp	Glicose monoidratada	12284230	1
sanacorp	Glicose monoidratada	13157026	1
Sanacorp	Glicose monoidratada	14102430	1
Sanacorp	Glicose monoidratada	1607024-01	1
Sanacorp	Glicose monoidratada	16184810	1
Sanacorp	Glicose monoidratada	17136804	1
Sanacorp	Glicose monoidratada	1807005-02	1
Sanacorp	Glicose monoidratada	18101903	2
Sanacorp	Glicose monoidratada	18101907	1
Sanacorp	Glicose monoidratada	1811020	1
Sanacorp	Glicose monoidratada	18214703	1
Sanacorp	Glicose monoidratada	18214704	1
Sanacorp	Glicose monoidratada	19073301	1
Sanacorp	Glicose monoidratada	19073303	1
sanacorp	Glicose monoidratada	19073304	1
Sanacorp	Glicose monoidratada	192486002	1
Sanacorp	Glicose monoidratada	20004182008	1
Sanacorp	Glicose monoidratada	2001006-01	1
Sanacorp	Glicose monoidratada	21001886009	1
sanacorp	Glicose monoidratada	2103027-01	1
Sanacorp	Glicose monoidratada	2107024-02	2
Sanacorp	Glicose monoidratada	22000756007	1
Sanacorp	Glicose monoidratada	22000756017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Glicose monoidratada	2202015-01	1
Sanacorp	Glicose monoidratada	2206018-01	2
Sanacorp	Glicose monoidratada	23000211001	1
Sanacorp	Glicose monoidratada	23000211005	1
Sanacorp	Glicose monoidratada	2310008-01	1
Sanacorp	Glicose monoidratada	3/AKD100	1
Sanacorp	Glicose monoidratada	E316T	1
Sanacorp	Glicose monoidratada	E388S	2
sittig	Glicose monoidratada	17005805	1
Sonnenberg-Apotheke	Glicose monoidratada	140500401	1

- 231 534 spectra from 1515 *Apo-Ident* customers from a total of 48 694 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glicose monoidratada* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glicose monoidratada* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	970	0	201 114
Type C	0	4525	8	231 534

The substance/substance group *Glicose monoidratada* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3814 %)
Type C	100.0000 % (> 99.9007 %)	99.8235 % (> 99.7573 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20799	22538	5,99	167,74
21274	21905	6,28	171,69
21905	21905	0,00	165,89
22308	22308	0,00	169,89
22538	22538	0,00	168,50
23006	23006	0,00	167,90
23304	23304	0,00	168,92
23802	23802	0,00	171,02
24162	24162	0,00	173,37
25627	25627	0,00	171,05
25637	25637	0,00	170,23
25653	25653	0,00	170,65

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gluconato de cálcio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20871-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gluconato de cálcio; Calcii gluconas; Glicinato de cálcio

Special notes

When selecting the *Gluconato de cálcio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gluconato de cálcio	6	9	82

Second-stage model

For differentiation of the substance/substance group *Gluconato de cálcio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gluconato de cálcio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	68,67	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gluconato de cálcio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gluconato de cálcio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Gluconato de cálcio	12236502	20871	40	1401575
Caelo	Gluconato de cálcio	12335829	21312	40	20121121
Euro OTC	Gluconato de cálcio	1304012-01	21283	40	AR-15-FG-008127-01
Euro OTC	Gluconato de cálcio	1407041-01	21821	60	20140818
Euro OTC	Gluconato de cálcio	1712007	23873	40	20171220*
Euro OTC	Gluconato de cálcio	1911017	25086	40	20200123*
Euro OTC	Gluconato de cálcio	1712007	25106	40	20200203*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Gluconato de cálcio*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 662 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 410 spectra of 12 reference samples from the substance/substance group *Gluconato de cálcio*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Gluconato de cálcio	154356	23360	40
Caelo	Gluconato de cálcio	181010	24017	40
Caelo	Gluconato de cálcio	190240	24566	40
Caelo	Gluconato de cálcio	20004137011	25986	40
Caelo	Gluconato de cálcio	22001257	26250	40
Caelo	Gluconato de cálcio	24000791	27223	40
Euro OTC	Gluconato de cálcio	1606034	22699	40
Euro OTC	Gluconato de cálcio	1905015	24791	40
Fagron	Gluconato de cálcio	22D13-B03-229458	26666	40
Caelo	Gluconato de cálcio	20004137011	25986SI	10
Caelo	Gluconato de cálcio	22001257	26250SI	20
Fagron	Gluconato de cálcio	22D13-B03-229458	26666SI	20

- 201 674 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 278 spectra from 160 *Apo-Ident* customers from 85 batches from the substance/substance group *Gluconato de cálcio*.

- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gluconato de cálcio	171200-02	1
	Gluconato de cálcio	21003557009	1
	Gluconato de cálcio	22001257002	2
	Gluconato de cálcio	22001257003	5
	Gluconato de cálcio	22001257006	4
	Gluconato de cálcio	22001257008	1
AHD	Gluconato de cálcio	1911017-03	1
AHD	Gluconato de cálcio	21003557007	1
apomix	Gluconato de cálcio	1905015-02	1
Berkel AHK	Gluconato de cálcio	14085407	2
Caelo	Gluconato de cálcio	1000041-01	1
Caelo	Gluconato de cálcio	12335810	1
Caelo	Gluconato de cálcio	12335813	1
Caelo	Gluconato de cálcio	1407041-01	1
Caelo	Gluconato de cálcio	140704102	1
Caelo	Gluconato de cálcio	1407041-02	1
Caelo	Gluconato de cálcio	14085405	1
Caelo	Gluconato de cálcio	14230706	1
Caelo	Gluconato de cálcio	15126301	1
Caelo	Gluconato de cálcio	15324806	1
Caelo	Gluconato de cálcio	15324807	1
Caelo	Gluconato de cálcio	15435601	2
Caelo	Gluconato de cálcio	15435607	2
Caelo	Gluconato de cálcio	15435610	1
Caelo	Gluconato de cálcio	15435611	1
Caelo	Gluconato de cálcio	15435613	1
Caelo	Gluconato de cálcio	15435619	4
Caelo	Gluconato de cálcio	15435620	2
Caelo	Gluconato de cálcio	15435622	2
Caelo	Gluconato de cálcio	1543601	1
Caelo	Gluconato de cálcio	1606034	1
Caelo	Gluconato de cálcio	1606034-01	1
Caelo	Gluconato de cálcio	16603401	1
Caelo	Gluconato de cálcio	171200-01	1
Caelo	Gluconato de cálcio	1712007_02	1
Caelo	Gluconato de cálcio	1712007-02	1
Caelo	Gluconato de cálcio	18101003	2
Caelo	Gluconato de cálcio	18101004	3
Caelo	Gluconato de cálcio	18101006	2
Caelo	Gluconato de cálcio	18101010	2
Caelo	Gluconato de cálcio	18106202	2
Caelo	Gluconato de cálcio	1900240002	1
Caelo	Gluconato de cálcio	190240001	2
Caelo	Gluconato de cálcio	190240002	10
Caelo	Gluconato de cálcio	19024006	5
Caelo	Gluconato de cálcio	19024009	2
Caelo	Gluconato de cálcio	190240096	1
Caelo	Gluconato de cálcio	1905015-01	1
Caelo	Gluconato de cálcio	190772007	1
Caelo	Gluconato de cálcio	19240002	1
Caelo	Gluconato de cálcio	20004137002	5
Caelo	Gluconato de cálcio	20004137004	1
Caelo	Gluconato de cálcio	20004137006	3
Caelo	Gluconato de cálcio	21003557007	2
Caelo	Gluconato de cálcio	22001257003	1
Caelo	Gluconato de cálcio	4(18101004)	1
Caesar & Loretz GmbH...	Gluconato de cálcio	20004137006	2
Caesar & Loretz GmbH	Gluconato de cálcio	19024006	2
Caesar & Loretz GmbH	Gluconato de cálcio	19024009	1
Caesar & Loretz GmbH	Gluconato de cálcio	20004137002	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Gluconato de cálcio	20004137005	1
Caesar & Loretz GmbH	Gluconato de cálcio	20004137006	1
Caesar & Loretz GmbH	Gluconato de cálcio	20004137011	2
Caesar & Loretz GmbH	Gluconato de cálcio	21003557007	1
Caesar&Lorenz/AHD	Gluconato de cálcio	19024009	1
Caleo/ Noweda	Gluconato de cálcio	18101004	2
Eurho/Sns	Gluconato de cálcio	1209006-01	1
EuRho	Gluconato de cálcio	12090006-01	1
EuRho	Gluconato de cálcio	1209006-01	2
EuRho	Gluconato de cálcio	1304012-01	1
Euro OTC	Gluconato de cálcio	1105027-01	1
Euro OTC	Gluconato de cálcio	1105027-02	3
Euro OTC	Gluconato de cálcio	115027-01	1
Euro OTC	Gluconato de cálcio	1209006-01	7
Euro OTC	Gluconato de cálcio	1210001287	1
Euro OTC	Gluconato de cálcio	1304012-01	6
Euro OTC	Gluconato de cálcio	130401202	1
Euro OTC	Gluconato de cálcio	1304012-02	2
Euro OTC	Gluconato de cálcio	140704101	1
Euro OTC	Gluconato de cálcio	1407041-01	6
Euro OTC	Gluconato de cálcio	140704102	1
Euro OTC	Gluconato de cálcio	1407041-02	9
Euro OTC	Gluconato de cálcio	1602001644	3
Euro OTC	Gluconato de cálcio	1606034-01	20
Euro OTC	Gluconato de cálcio	1606034-02	10
Euro OTC	Gluconato de cálcio	1702000290	1
Euro OTC	Gluconato de cálcio	1712007	1
Euro OTC	Gluconato de cálcio	1712007-01	11
Euro OTC	Gluconato de cálcio	1712007-02	11
Euro OTC	Gluconato de cálcio	1712007-03	1
Euro OTC	Gluconato de cálcio	1712007-04	11
Euro OTC	Gluconato de cálcio	1905015-01	16
Euro OTC	Gluconato de cálcio	1905015-02	11
Euro OTC	Gluconato de cálcio	1911017-01	1
Euro OTC	Gluconato de cálcio	20270912-1	1
Euro OTC	Gluconato de cálcio	513-Q1211	1
Euro/Gehe	Gluconato de cálcio	1304012-01	1
Fagron	Gluconato de cálcio	10G22-N12	1
Fagron	Gluconato de cálcio	12D17-N01	1
Fagron	Gluconato de cálcio	14D11-B04	1
Fagron	Gluconato de cálcio	14D11-B04-294136	2
Fagron	Gluconato de cálcio	15D13-B98-307445	1
Fagron	Gluconato de cálcio	17E30-B02-343011	1
Finze	Gluconato de cálcio	917857359	1
Gatt-Koller / Phoenix	Gluconato de cálcio	550/03141214	1
Gehe/EuRo	Gluconato de cálcio	1712007-01	1
GEHE	Gluconato de cálcio	15435619	1
Gehe	Gluconato de cálcio	20004137011	1
L12	Gluconato de cálcio	15435627	1
Noweda	Gluconato de cálcio	15435627	1
Pharmachem	Gluconato de cálcio	18101003	1
Phönix/Euro	Gluconato de cálcio	1606034-01	1
Phönix	Gluconato de cálcio	1606034-01	1
sanacorp	Gluconato de cálcio	1407041-01	1
Sidonia	Gluconato de cálcio	18101004	1

- 235 789 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gluconato de cálcio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gluconato de cálcio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	410	0	201 674
Type C	0	278	0	235 789

The substance/substance group *Gluconato de cálcio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5366 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.8417 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20871	20871	0,00	151,25
21283	21283	0,00	143,28
21312	20871	11,02	151,89
21821	23873	3,80	142,14
23873	23873	0,00	141,97
25086	25086	0,00	155,09
25106	25106	0,00	144,98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gluconato de zinco**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20379-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gluconato de zinco; Glicinato de zinco; Zinci gluconas

Special notes

When selecting the *Gluconato de zinco* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gluconato de zinco	8	17	56

Second-stage model

For differentiation of the substance/substance group *Gluconato de zinco* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gluconato de zinco* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	55,50	–
⋮	⋮	⋮
Sulfato de tobramicina	>50	28,46
Sulfato de neomicina	>50	55,29
Fosfato sódico de riboflavina hidratado	>50	55,50
Sulfato de gentamicina	>50	74,50
Citrato de magnésio	>50	85,11
Carbômero	>50	117,96
Fosfato de Mg-Ca-K-colamina	>50	122,17
Tetraborato de sódio	>50	302,29
Finasterida	>50	1654,12

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gluconato de zinco* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gluconato de zinco*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Gluconato de zinco	170165	23034	40	20170125*
Caelo	Gluconato de zinco	170951	23292	40	20170518*
Euro OTC	Gluconato de zinco	1407033-02	21709	60	20140902
Euro OTC	Gluconato de zinco	1508007	21882	60	20150827*
Euro OTC	Gluconato de zinco	1603035	22513	40	20160427*
Euro OTC	Gluconato de zinco	1807019	24150	40	20180725*
Euro OTC	Gluconato de zinco	2007007	25318	40	20200826*
Euro OTC	Gluconato de zinco	2103006	25603	40	20210323*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Gluconato de zinco*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 21 reference samples from the substance/substance group *Gluconato de zinco*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Gluconato de zinco	161788	22619	40
Caelo	Gluconato de zinco	20002679	25611	40
Caelo	Gluconato de zinco	23001539	26893	40
Euro OTC	Gluconato de zinco	1606018	22700	40
Euro OTC	Gluconato de zinco	1701017	22994	40
Euro OTC	Gluconato de zinco	1706009	23544	40
Euro OTC	Gluconato de zinco	1711004	23730	40
Euro OTC	Gluconato de zinco	1810014	24347	40
Euro OTC	Gluconato de zinco	1902017	24635	40
Euro OTC	Gluconato de zinco	1910010	24942	40
Euro OTC	Gluconato de zinco	2007027	25316	40
Euro OTC	Gluconato de zinco	2110001	25887	50
Euro OTC	Gluconato de zinco	2208029	26338	40
Euro OTC	Gluconato de zinco	2302019	26641	40
Euro OTC	Gluconato de zinco	2312003	27074	40
Euro OTC	Gluconato de zinco	2405017	27293	40
Fagron	Gluconato de zinco	22L30-B04-225958	26919	40
Caelo	Gluconato de zinco	23001539	26893SI	20
Euro OTC	Gluconato de zinco	2110001	25887SI	10
Euro OTC	Gluconato de zinco	2208029	26338SI	20
Euro OTC	Gluconato de zinco	2302019	26641SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 324 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 447 spectra from 22 *Apo-Ident* customers from 58 batches from the substance/substance group *Gluconato de zinco*.

- Among them are spectra of independent samples from 56 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gluconato de zinco	2312003-01	1
	Gluconato de zinco	23C22-B09	2
	Gluconato de zinco	7500200698	1
Caelo	Gluconato de zinco	16001601	1
Caelo	Gluconato de zinco	16178801	1
Caelo	Gluconato de zinco	17016502	3
Caelo	Gluconato de zinco	17095103	1
Caelo	Gluconato de zinco	18069506	1
Caelo	Gluconato de zinco	18069511	1
Caelo	Gluconato de zinco	19044602	3
Caelo	Gluconato de zinco	19044603	2
Caelo	Gluconato de zinco	19044607	1
Caelo	Gluconato de zinco	191451002	1
Caelo	Gluconato de zinco	19145103	1
Caelo	Gluconato de zinco	20000647001	1
Caelo	Gluconato de zinco	20000647002	1
Caelo	Gluconato de zinco	20002679003	1
Caelo	Gluconato de zinco	20002679004	1
Caelo	Gluconato de zinco	20003987	1
Caelo	Gluconato de zinco	20003987001	3
Caelo	Gluconato de zinco	20003987002	1
Caelo	Gluconato de zinco	20003987005	1
Caelo	Gluconato de zinco	21003511001	3
Caelo	Gluconato de zinco	21003511003	2
Caelo	Gluconato de zinco	22003957003	3
Caelo	Gluconato de zinco	23001539001	1
Caelo	Gluconato de zinco	23003413002	1
Caesar & Loretz GmbH	Gluconato de zinco	19044607	1
Caesar & Loretz GmbH	Gluconato de zinco	20003987004	1
Euro OTC	Gluconato de zinco	1312010-01	1
Euro OTC	Gluconato de zinco	1405011-01	1
Euro OTC	Gluconato de zinco	1508007-01	16
Euro OTC	Gluconato de zinco	1508007-02	40
Euro OTC	Gluconato de zinco	1603035-01	40
Euro OTC	Gluconato de zinco	1606018-01	34
Euro OTC	Gluconato de zinco	1606018-02	36
Euro OTC	Gluconato de zinco	1701017-01	31
Euro OTC	Gluconato de zinco	1706009-01	66
Euro OTC	Gluconato de zinco	170901201	9
Euro OTC	Gluconato de zinco	1709012-0103707875	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Gluconato de zinco	1711004-01	28
Euro OTC	Gluconato de zinco	1807019	1
Euro OTC	Gluconato de zinco	1807019-01	14
Euro OTC	Gluconato de zinco	1810014-01	29
Euro OTC	Gluconato de zinco	1902017-01	1
Euro OTC	Gluconato de zinco	1902018-01	5
Euro OTC	Gluconato de zinco	191001001	1
Euro OTC	Gluconato de zinco	1910010-01	2
Euro OTC	Gluconato de zinco	2007007	1
Euro OTC	Gluconato de zinco	2007007-01	6
Euro OTC	Gluconato de zinco	2007027-01	19
Euro OTC	Gluconato de zinco	2103006-01	9
Euro OTC	Gluconato de zinco	211000101	1
Euro OTC	Gluconato de zinco	2110001-01	8
Euro OTC	Gluconato de zinco	27061711	1
Euro OTC	Gluconato de zinco	ZGE-USP2004028	1
Fagron	Gluconato de zinco	14J30-B06-300520	1
Fagron	Gluconato de zinco	20G06-F01-372826	1
Fagron	Gluconato de zinco	22A21-B08-216993	1

- 235 620 spectra from 1515 *Apo-Ident* customers from a total of 49 201 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gluconato de zinco* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gluconato de zinco* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	760	0	201 324
Type C	0	447	0	235 620

The substance/substance group *Gluconato de zinco* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6577 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21709	25603	5,52	63,42
21882	21882	0,00	63,84
22513	22513	0,00	72,05
23034	23034	0,00	61,33
23292	23292	0,00	61,85
24150	24150	0,00	69,83
25318	25318	0,00	61,76
25603	25603	0,00	66,11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gluconato ferroso hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24166-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gluconato ferroso hidratado; Ferrosi gluconas hydricus; Glicinato ferroso hidratado

Special notes

When selecting the *Gluconato ferroso hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gluconato ferroso hidratado	4	1	0

Second-stage model

For differentiation of the substance/substance group *Gluconato ferroso hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gluconato ferroso hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	108,35	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gluconato ferroso hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gluconato ferroso hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Gluconato ferroso hidratado	2008035	25378	40	20201015*
Euro OTC	Gluconato ferroso hidratado	2103004	25604	40	20210329*
Euro OTC	Gluconato ferroso hidratado	2201008	26085	40	20220425*
Euro OTC	Gluconato ferroso hidratado	2307024	26859	40	20230821*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Gluconato ferroso hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 802 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Gluconato ferroso hidratado*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Gluconato ferroso hidratado	1805025	24166	40
Euro OTC	Gluconato ferroso hidratado	2201008	26085SI†	20
Euro OTC	Gluconato ferroso hidratado	2307024	26859SI†	20

- 202 004 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Gluconato ferroso hidratado*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Gluconato ferroso hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gluconato ferroso hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Gluconato ferroso hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25378	25378	0,00	410,06
25604	25604	0,00	400,53
26085	26085	0,00	401,96
26859	26859	0,00	400,04

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glutamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	23150-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glutamina; Glutaminum

Special notes

When selecting the *Glutamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glutamina	6	7	1

Second-stage model

For differentiation of the substance/substance group *Glutamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glutamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	113,88	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glutamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glutamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glutamina	1702007	23150	40	20170322*
Euro OTC	Glutamina	1706010	23543	40	20170802*
Euro OTC	Glutamina	2003034	25238	40	20200619*
Euro OTC	Glutamina	2006029	25347	40	20200813*
Euro OTC	Glutamina	2011010	25458	40	20201208*
Fagron	Glutamina	17E05-B06-334869	23415	40	20170601
Fagron	Glutamina	17E05-B06-334869	23416	40	AR-17-FG-016178-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 7 reference samples from the substance/substance group *Glutamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 330 spectra of 9 reference samples from the substance/substance group *Glutamina*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glutamina	1802010	23950	40
Euro OTC	Glutamina	1806001	24121	40
Euro OTC	Glutamina	1901009	24483	40
Euro OTC	Glutamina	2101010	25576	40
Euro OTC	Glutamina	2108006	25773	50
Euro OTC	Glutamina	2205028	26224	40
Euro OTC	Glutamina	2301005	26519	40
Euro OTC	Glutamina	2205028	26224SI	20
Euro OTC	Glutamina	2301005	26519SI	20

- 201 754 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Glutamina*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Glutamina	1706010-01	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glutamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glutamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	330	0	201 754
Type C	0	1	0	236 066

The substance/substance group *Glutamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1818 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23150	23150	0,00	205,25
23415	23416	1,74	211,62
23416	23416	0,00	211,34
23543	23543	0,00	204,82
25238	25238	0,00	205,77
25347	25347	0,00	208,49
25458	25458	0,00	210,93

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glutationa**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20366-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glutationa

Special notes

When selecting the *Glutationa* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glutationa	7	7	12

Second-stage model

For differentiation of the substance/substance group *Glutationa* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glutationa* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	80,43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glutationa* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glutationa*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glutationa	1102019-02	21788	60	AR-15-FG-008218-01
Euro OTC	Glutationa	1703008	23143	40	20170327*
Euro OTC	Glutationa	1808036	24314	40	20180919*
Euro OTC	Glutationa	2002042	25250	40	20200622*
Euro OTC	Glutationa	2007021	25337	40	20200810*
Euro OTC	Glutationa	2306012	27069	40	20240208*
Euro OTC	Glutationa	2306012	27069SI	20	20240208*
Fagron	Glutationa	18C01-B08-347604	24059	40	20180416

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Glutationa*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 300 spectra of 8 reference samples from the substance/substance group *Glutationa*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glutationa	1711009	23729	40
Euro OTC	Glutationa	1901052	24491	40
Euro OTC	Glutationa	1905011	24675	40
Euro OTC	Glutationa	2105017	25680	40
Euro OTC	Glutationa	2205027	26436	40
Fagron	Glutationa	19B04-B04-365527	25439	40
Fagron	Glutationa	22K21-B03-230393	26978	40
Fagron	Glutationa	22K21-B03-230393	26978SI	20

- 201 784 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 25 spectra from 5 *Apo-Ident* customers from 12 batches from the substance/substance group *Glutationa*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Changsha Huir	Glutationa	2201190	1
Euro OTC	Glutationa	1905011-01	1
Euro OTC	Glutationa	2002042-01	13
Fagron	Glutationa	14H21-B02	1
Farmalabor	Glutationa	P1700811	1
Shangei tengben Biot…	Glutationa	B210411	1
Vivatis Pharma	Glutationa	B200617	1
Vivatis Pharma	Glutationa	B210107	1
Vivatis Pharma	Glutationa	B210115	1
Vivatis Pharma	Glutationa	B210413	2
Vivatis Pharma	Glutationa	B210530	1
Vivatis Pharma	Glutationa	B220117	1

- 236 042 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glutationa* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glutationa* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	300	0	201 784
Type C	0	25	0	236 042

The substance/substance group *Glutationa* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 76.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21788	21788	0,00	165,93
23143	23143	0,00	170,71
24059	27069	8,46	174,74
24314	24314	0,00	148,28
25250	25250	0,00	160,54
25337	25337	0,00	163,28
27069	27069	0,00	167,08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Goma arábica, dispersão seca**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20457-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Goma arábica, dispersão seca; Acaciae gummi dispersione desiccatum

Special notes

When selecting the *Goma arábica, dispersão seca* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Goma arábica, dispersão seca	6	3	13

Second-stage model

For differentiation of the substance/substance group *Goma arábica, dispersão seca* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Goma arábica, dispersão seca* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
SyrSpend® SF pH4	31,08	14,74
SyrSpend® SF Alka	36,52	24,69
Amido de arroz	42,29	25,18
SyrSpend® SF pH4 neo	43,81	16,10
Amido de trigo	52,59	21,57
⋮	⋮	⋮
Carmelose sódica	>50	23,78
Amido de milho	>50	26,09
Sulfato de colistina	>50	29,02
Sulfato de polimixina B	>50	32,08
Maltodextrina	>50	32,18
Glicerofosfato de cálcio	>50	32,56
Fécula de batata	>50	33,46
Anfotericina B	>50	45,81
Cianocobalamina	>50	48,78
Bacitracina	>50	52,95
Riboflavina	>50	60,82
Levedura de selênio	>50	68,14
Tosilcloramida sódica	>50	81,31
Pantotenato de cálcio	>50	84,12
Nistatina	>50	85,74
Ácido oxálico	>50	92,52
Frutose	>50	97,16
Gelatina, branca	>50	102,27
Bromidrato de hioscina	>50	108,17
Estradiol hemi-hidratado	>50	132,23
Triancinolona	>50	132,79
Vitamina E acetato pó 50%	>50	133,00
Estriol	>50	169,90
Metilcobalamina	>50	173,29

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Goma arábica, dispersão seca* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Goma arábica, dispersão seca*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Goma arábica, dispersão seca	14141901	21431	120	AR-15-FG-006809-01
Caelo	Goma arábica, dispersão seca	15413201	22653	40	AR-17-FG-000844-01
Caelo	Goma arábica, dispersão seca	181860	24730	40	20180725*
Caelo	Goma arábica, dispersão seca	192248013	25501	40	20190828
Caelo	Goma arábica, dispersão seca	24001100	27261	40	20240604*
Caelo	Goma arábica, dispersão seca	24002524	27443	40	20241105*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 6 reference samples from the substance/substance group *Goma arábica, dispersão seca*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 7 reference samples from the substance/substance group *Goma arábica, dispersão seca*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Goma arábica, dispersão seca	162331	22853	40
Caelo	Goma arábica, dispersão seca	16233105	23443	40
Caelo	Goma arábica, dispersão seca	21003060	25982	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Goma arábica, dispersão seca	16233105	23444	40
Caelo	Goma arábica, dispersão seca	21003060	25982SI	10
Caelo	Goma arábica, dispersão seca	24001100	27261SI†	20
Caelo	Goma arábica, dispersão seca	24002524	27443SI†	20

- 201 874 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 13 *Apo-Ident* customers from 14 batches from the substance/substance group *Goma arábica, dispersão seca*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Goma arábica, dispersão seca	11345715	1
Caelo	Goma arábica, dispersão seca	12111301	1
Caelo	Goma arábica, dispersão seca	12138607	1
Caelo	Goma arábica, dispersão seca	12138612	1
Caelo	Goma arábica, dispersão seca	12372302	1
Caelo	Goma arábica, dispersão seca	15086704	1
Caelo	Goma arábica, dispersão seca	15413201	1
Caelo	Goma arábica, dispersão seca	15413207	1
Caelo	Goma arábica, dispersão seca	16233105	2
Caelo	Goma arábica, dispersão seca	21003060011	1
Caelo	Goma arábica, dispersão seca	3314A160121	1
Caesar & Loretz GmbH	Goma arábica, dispersão seca	18186001	1
Klenk	Goma arábica, dispersão seca	3314A140121	1
ROHA	Goma arábica, dispersão seca	170190	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Goma arábica, dispersão seca* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Goma arábica, dispersão seca* and it was evaluated how many matches (positive) and rejections (negative) were correct or

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	210	0	201 874
Type C	0	15	0	236 052

The substance/substance group *Goma arábica, dispersão seca* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21431	21431	0,00	41,92
22653	22653	0,00	36,02
24730	24730	0,00	39,77
25501	22653	6,70	38,18
27261	27261	0,00	35,33
27443	27443	0,00	37,13

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gramicidina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20203-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gramicidina; Gramicidinum

Special notes

When selecting the *Gramicidina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gramicidina	6	3	9

Second-stage model

For differentiation of the substance/substance group *Gramicidina* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gramicidina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	65,67	–
⋮	⋮	⋮
Tirotricina	>50	52,43
Fluocinolona acetonida	>50	99,37
Metilprednisolona	>50	99,68
Triancinolona acetonido	>50	104,32
Prednisolona	>50	125,28
Betametasona	>50	165,20
Dexametasona	>50	169,13

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gramicidina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gramicidina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Gramicidina	13J15-N02	21253	40	AR-15-FG-000813-01
Fagron	Gramicidina	17E09-B02-341211	23744	40	AR-18-FG-008970-02
Fagron	Gramicidina	18A19-B14-350428	24171	40	20180704
Fagron	Gramicidina	18L20-B01-358528	24571	40	20190320
Fagron	Gramicidina	19D30-B01-195185	25181	40	20190619
Fagron	Gramicidina	21G10-B12-213720	26326	40	20210928
Fagron	Gramicidina	21G10-B12-213720	26326SI	20	20210928

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 7 reference samples from the substance/substance group *Gramicidina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Gramicidina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Gramicidina	14C07-B06-292886	21544	40
Fagron	Gramicidina	15H18-B01-316269	22748	40
Fagron	Gramicidina	20I29-B07-200272	25587	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 7 *Apo-Ident* customers from 11 batches from the substance/substance group *Gramicidina*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Gramicidina		1
Fagron	Gramicidina	11F-24-N03	1
Fagron	Gramicidina	12K22-N12	1
Fagron	Gramicidina	14H06-B03-297614	2
Fagron	Gramicidina	15C11-B04-306766	1
Fagron	Gramicidina	15H18B01316269	1
Fagron	Gramicidina	17E09-B02-341211	1
Fagron	Gramicidina	20129-B07-200272	1
Fagron	Gramicidina	20I29B07200272	1
Fagron	Gramicidina	21G10B12213720	1
Fagron	Gramicidina	B3200266	1

- 236 055 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gramicidina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gramicidina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	120	0	201 964
Type C	0	12	0	236 055

The substance/substance group *Gramicidina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21253	21253	0,00	114,94
23744	23744	0,00	118,00
24171	23744	4,74	117,96
24571	21253	9,12	128,15
25181	23744	4,93	124,45
26326	23744	6,15	125,34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Griseofulvina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20939-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Griseofulvina; Griseofulvinum

Special notes

When selecting the *Griseofulvina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Griseofulvina	4	2	61

Second-stage model

For differentiation of the substance/substance group *Griseofulvina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Griseofulvina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Brometo de neostigmina	101,61	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Griseofulvina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Griseofulvina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Griseofulvina	13D19-N03	20939	40	1401419
Fagron	Griseofulvina	14E16-B01-296834	21725	60	20140526
Fagron	Griseofulvina	16F13-B06-330832	23594	40	20160713
Fagron	Griseofulvina	22K14-B07-213300	26459	40	20221123
Fagron	Griseofulvina	22K14-B07-213300	26459SI	20	20221123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Griseofulvina*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 762 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Griseofulvina*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Griseofulvina	17L05-B05-345995	23996	40
Fagron	Griseofulvina	18L04_B01-357660	24440	40

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 134 spectra from 51 *Apo-Ident* customers from 67 batches from the substance/substance group *Griseofulvina*.
- Among them are spectra of independent samples from 61 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD	Griseofulvina	17L05-B05-349129	1
AHD	Griseofulvina	18L04-B01-357660	1
AHD	Griseofulvina	18L04-B01-361614	1
AHD	Griseofulvina	18Lo4-B01-357660	1
AHD	Griseofulvina	B01-3616104	1
Alliance Healthcare	Griseofulvina	18L04-B01-363841	1
Bombastus	Griseofulvina	15L03-HH150640	1
Bombastus	Griseofulvina	16F13-B06-326073	1
Bombastus	Griseofulvina	17L05-B05-345996	1
Caelo	Griseofulvina	100910	1
Caelo	Griseofulvina	16F13-B06-323068	1
Caelo	Griseofulvina	16F13-B06-326074	1
Caelo	Griseofulvina	16F13-B06-330833	1
Euro OTC	Griseofulvina		1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Griseofulvina	14E16-B01-300367	1
Fagron	Griseofulvina	10F03-N12	1
Fagron	Griseofulvina	11J11-N13	1
Fagron	Griseofulvina	12D04-N12	1
Fagron	Griseofulvina	12F18-N04	1
Fagron	Griseofulvina	130922	2
Fagron	Griseofulvina	13D19-N03	1
Fagron	Griseofulvina	13F12-N22	1
Fagron	Griseofulvina	13L13-B08	1
Fagron	Griseofulvina	13L-13B08	1
Fagron	Griseofulvina	13L13-B08-290316	4
Fagron	Griseofulvina	13L13-B08-290317	1
Fagron	Griseofulvina	140410	2
Fagron	Griseofulvina	14E16-B01-300366	3
Fagron	Griseofulvina	14E16-B01-300367	1
Fagron	Griseofulvina	15062015A	1
Fagron	Griseofulvina	15810-B06	1
Fagron	Griseofulvina	15B10-B06	1
Fagron	Griseofulvina	15B10-B06-306547	9
Fagron	Griseofulvina	15B10-B06-306663	1
Fagron	Griseofulvina	15B10-B06-396547	1
Fagron	Griseofulvina	15l03-b04-315624	1
Fagron	Griseofulvina	15L03-B04-315624	3
Fagron	Griseofulvina	15L03-B315624	1
Fagron	Griseofulvina	16F13-B06	1
Fagron	Griseofulvina	16F13-B06-323067	3
Fagron	Griseofulvina	16F13-B06-323068	2
Fagron	Griseofulvina	16F13-B06-326073	1
Fagron	Griseofulvina	16f13-b06-326074	1
Fagron	Griseofulvina	16F13-B06-330832	5
Fagron	Griseofulvina	16f13-b06-330833	1
Fagron	Griseofulvina	16F13B06330833	1
Fagron	Griseofulvina	16F13-B06-330833	5
Fagron	Griseofulvina	17-L05-352461	1
Fagron	Griseofulvina	17L05-B05	5
Fagron	Griseofulvina	17L05-B05-345995	3
Fagron	Griseofulvina	17L05-B05-34999	1
Fagron	Griseofulvina	17L05-B05-351232	4
Fagron	Griseofulvina	17L05B05352461	2
Fagron	Griseofulvina	17L05-B05-352461	3
Fagron	Griseofulvina	17L05-B05-355075	1
Fagron	Griseofulvina	17LO05-B05-352461	1
Fagron	Griseofulvina	17LO5-BO5	1
Fagron	Griseofulvina	17LO5-BO5-352461	1
Fagron	Griseofulvina	17LOS-B05-351232	1
Fagron	Griseofulvina	18L04-B01	2
Fagron	Griseofulvina	18L04-B01-357660	3
Fagron	Griseofulvina	18L04-B01-357661	1
Fagron	Griseofulvina	18L04-B01-359072	2
Fagron	Griseofulvina	18L04-B01-359073	2
Fagron	Griseofulvina	18L04-B01-361614	4
Fagron	Griseofulvina	18L04-B01-361615	3
Fagron	Griseofulvina	18L04-B01-3670033	1
Fagron	Griseofulvina	18LO4-BO1-357660	1
Fagron	Griseofulvina	B01-3670303	1
Fagron	Griseofulvina	HH160510	1
Fagron	Griseofulvina	HH171022	1
Fargon GmbH & Co.KG	Griseofulvina	16F13-B06-323067	1
Fargon/Sanacorp	Griseofulvina	17L05-B05-351231	1
Gehe	Griseofulvina	15B10-B06-306547	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
LAP	Griseofulvina	15L03-B04-315624	1
Noweda	Griseofulvina	16F13-B06-330833	1
Noweda	Griseofulvina	17L05-B05-345995	2
Phönix Gotha	Griseofulvina	140410	1
Sanacorp Stralsund	Griseofulvina	18L04-B01-359073	2
Sanacorp/ F	Griseofulvina	12B06-N07	1
Sanacorp	Griseofulvina	17L05-B05-345995	1

- 235 933 spectra from 1515 *Apo-Ident* customers from a total of 49 192 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Griseofulvina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Griseofulvina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	80	0	202 004
Type C	0	120	14	235 933

The substance/substance group *Griseofulvina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	89.5522 % (> 87.3134 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20939	20939	0,00	120,54
21725	20939	14,16	122,42
23594	20939	7,81	129,71
26459	20939	10,80	129,77

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Guaifenesina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20551-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Guaifenesina; Éter gliceril guaiacol; Guaifenesinum

Special notes

When selecting the *Guaifenesina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Guaifenesina	8	14	19

Second-stage model

For differentiation of the substance/substance group *Guaifenesina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Guaifenesina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	75,64	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Guaifenesina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Guaifenesina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Guaifenesina	163333	23051	40	20161221*
Caelo	Guaifenesina	172496	23644	40	20171005*
Euro OTC	Guaifenesina	1212002-01	21287	40	20121214
Euro OTC	Guaifenesina	1506044	21864	60	20150708*
Euro OTC	Guaifenesina	1605005	22555	40	20160525*
Euro OTC	Guaifenesina	1910023	24941	40	20191114*
Euro OTC	Guaifenesina	2206012	26219	40	20220715*
Euro OTC	Guaifenesina	2206012	26219SI	20	20220715*
Fagron	Guaifenesina	22H03-B01-227258	26549	40	20220823
Fagron	Guaifenesina	22H03-B01-227258	26549SI	20	20220823

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Guaifenesina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 582 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 580 spectra of 15 reference samples from the substance/substance group *Guaifenesina*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Guaifenesina	190134	24518	40
Euro OTC	Guaifenesina	1701011	22993	40
Euro OTC	Guaifenesina	1706006	23551	40
Euro OTC	Guaifenesina	1710033	23741	40
Euro OTC	Guaifenesina	1802001	23949	40
Euro OTC	Guaifenesina	1804004	24076	40
Euro OTC	Guaifenesina	1809011	24316	40
Euro OTC	Guaifenesina	1901047	24474	40
Euro OTC	Guaifenesina	1906008	24801	40
Euro OTC	Guaifenesina	2007006	25245	40
Euro OTC	Guaifenesina	2002034	25292	40
Euro OTC	Guaifenesina	2102012	25601	40
Euro OTC	Guaifenesina	2306003	26770	40
Euro OTC	Guaifenesina	2406001	27280	40
Euro OTC	Guaifenesina	2306003	26770SI	20

- 201 504 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 29 spectra from 9 *Apo-Ident* customers from 20 batches from the substance/substance group *Guaifenesina*.

- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Guaifenesina	1212002-01	1
Caelo	Guaifenesina	12277307	1
Caelo	Guaifenesina	12277311	1
Caelo	Guaifenesina	15302502	1
Caelo	Guaifenesina	15F30-b06-317816	1
Caelo	Guaifenesina	16135507	1
Caelo	Guaifenesina	1706006	1
Caelo	Guaifenesina	18018302	1
Euro OTC	Guaifenesina	1701011-01	1
Euro OTC	Guaifenesina	1706006-01	3
Euro OTC	Guaifenesina	1804004-01	1
Euro OTC	Guaifenesina	1809011-01	2
Euro OTC	Guaifenesina	18GF06347	1
Euro OTC	Guaifenesina	1906008-01	4
Euro OTC	Guaifenesina	1910023-01	1
Euro OTC	Guaifenesina	2002034-01	1
Euro OTC	Guaifenesina	2007006-01	3
Euro OTC	Guaifenesina	2102012-01	1
Euro OTC	Guaifenesina	2206012-01	1
Phoenix 05.07.2014	Guaifenesina	1402023-01	2

- 236 038 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Guaifenesina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Guaifenesina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	580	0	201 504
Type C	0	29	0	236 038

The substance/substance group *Guaifenesina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9655 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 79.3103 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21287	21864	16,40	240,63
21864	21864	0,00	240,72
22555	22555	0,00	236,50
23051	23051	0,00	242,20
23644	23644	0,00	241,81
24941	24941	0,00	241,92
26219	26219	0,00	239,87
26549	23051	5,54	241,41

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hemifumarato de colina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20719-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hemifumarato de colina; Cholinium bitartaricum; Colina, hemifumarato

Special notes

When selecting the *Hemifumarato de colina* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hemifumarato de colina	7	6	5

Second-stage model

For differentiation of the substance/substance group *Hemifumarato de colina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hemifumarato de colina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	150,12	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hemifumarato de colina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hemifumarato de colina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Hemifumarato de colina	1603044	22549	40	20160429*
Euro OTC	Hemifumarato de colina	1607020	22689	40	20160808*
Euro OTC	Hemifumarato de colina	1603044-01	23010	40	20160429
Euro OTC	Hemifumarato de colina	1603044-01	23101	40	20160429
Euro OTC	Hemifumarato de colina	1702005	23130	40	20170307*
Euro OTC	Hemifumarato de colina	1901053	24484	40	20190228*
Euro OTC	Hemifumarato de colina	1910013	24922	40	20191107*
Euro OTC	Hemifumarato de colina	2009020	25419	40	20200925*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Hemifumarato de colina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 260 spectra of 7 reference samples from the substance/substance group *Hemifumarato de colina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Hemifumarato de colina	1707023	23610	40
Euro OTC	Hemifumarato de colina	1711022	23903	40
Euro OTC	Hemifumarato de colina	1802008	23958	40
Euro OTC	Hemifumarato de colina	2006031	25303	40
Euro OTC	Hemifumarato de colina	2101036	25567	40
Euro OTC	Hemifumarato de colina	2110006	25872	50
Euro OTC	Hemifumarato de colina	2110006	25872SI	10

- 201 824 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 4 *Apo-Ident* customers from 6 batches from the substance/substance group *Hemifumarato de colina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Anzag/ Euro OT	Hemifumarato de colina	1910013-01	1
Euro OTC	Hemifumarato de colina	1309023-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Hemifumarato de colina	1603044-01	1
Euro OTC	Hemifumarato de colina	1607020-01	2
Euro OTC	Hemifumarato de colina	1707023-01	1
Euro OTC	Hemifumarato de colina	1711022-01	1

- 236 059 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hemifumarato de colina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hemifumarato de colina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	260	0	201 824
Type C	0	8	0	236 059

The substance/substance group *Hemifumarato de colina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22549	22549	0,00	270,03
22689	22689	0,00	272,54

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23010	22549	5,23	272,81
23101	22549	5,27	271,58
23130	23130	0,00	289,84
24484	24484	0,00	278,30
24922	24922	0,00	281,25
25419	25419	0,00	283,77

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hemissuccinato de doxilamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20315-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hemissuccinato de doxilamina; Doxylamini hydrogenosuccinas

Special notes

When selecting the *Hemissuccinato de doxilamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hemissuccinato de doxilamina	6	6	72

Second-stage model

For differentiation of the substance/substance group *Hemissuccinato de doxilamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hemissuccinato de doxilamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de benzidamina	82,86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hemissuccinato de doxilamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hemissuccinato de doxilamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hemissuccinato de doxilamina	15203906	23085	40	20151112
Caelo	Hemissuccinato de doxilamina	15203906	23086	40	20151112
Caelo	Hemissuccinato de doxilamina	183312	24535	40	20190219*
Fagron	Hemissuccinato de doxilamina	14F03-B01-293498	21542	60	1410524
Fagron	Hemissuccinato de doxilamina	15F01-B04-309189	22601	40	AR-16-FG-011361-01
Fagron	Hemissuccinato de doxilamina	20B19-F06-370985	25518	40	20200320
Fagron	Hemissuccinato de doxilamina	20K05-F03-375371	25838	50	20201207

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 310 spectra of 7 reference samples from the substance/substance group *Hemissuccinato de doxilamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 652 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 300 spectra of 9 reference samples from the substance/substance group *Hemissuccinato de doxilamina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hemissuccinato de doxilamina	172047	23626	40
Caelo	Hemissuccinato de doxilamina	181277	24536	40
Caelo	Hemissuccinato de doxilamina	20002147003	25514	40
Caelo	Hemissuccinato de doxilamina	22000214	26114	40
Caelo	Hemissuccinato de doxilamina	23003003	27119	40
Caelo	Hemissuccinato de doxilamina	24000843	27239	40
Caelo	Hemissuccinato de doxilamina	22000214	26114SI	20
Caelo	Hemissuccinato de doxilamina	23003003	27119SI	20
Caelo	Hemissuccinato de doxilamina	24000843	27239SI	20

- 201 784 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 166 spectra from 32 *Apo-Ident* customers from 74 batches from the substance/substance group *Hemissuccinato de doxilamina*.

- Among them are spectra of independent samples from 68 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hemissuccinato de doxilamina	B06_2286708	1
Caelo	Hemissuccinato de doxilamina		1
Caelo	Hemissuccinato de doxilamina	14k27-B07	1
Caelo	Hemissuccinato de doxilamina	15F01-B04-317385	2
Caelo	Hemissuccinato de doxilamina	15K04B01327356	1
Caelo	Hemissuccinato de doxilamina	16F06-B02-338804	2
Caelo	Hemissuccinato de doxilamina	16F06-B02-357986	1
Caelo	Hemissuccinato de doxilamina	18331201	1
Caelo	Hemissuccinato de doxilamina	18331206	1
Caelo	Hemissuccinato de doxilamina	21C19-F04-377749	1
Caesar & Loretz GmbH...	Hemissuccinato de doxilamina	13A04-N02	4
Euro OTC	Hemissuccinato de doxilamina	16F06-B02-348869	1
Fagron	Hemissuccinato de doxilamina		5
Fagron	Hemissuccinato de doxilamina	11G20-N10	1
Fagron	Hemissuccinato de doxilamina	11K17-N04	3
Fagron	Hemissuccinato de doxilamina	12811328003	1
Fagron	Hemissuccinato de doxilamina	12811420001	1
Fagron	Hemissuccinato de doxilamina	12811625003	6
Fagron	Hemissuccinato de doxilamina	12E04-N04	3
Fagron	Hemissuccinato de doxilamina	12G10-N03	6
Fagron	Hemissuccinato de doxilamina	12K21-N01	2
Fagron	Hemissuccinato de doxilamina	13/26-N14	1
Fagron	Hemissuccinato de doxilamina	13A04-N02	3
Fagron	Hemissuccinato de doxilamina	13E29-N03	4
Fagron	Hemissuccinato de doxilamina	14F03B01293498	1
Fagron	Hemissuccinato de doxilamina	14F03-B01-296845	1
Fagron	Hemissuccinato de doxilamina	14K27-B07	1
Fagron	Hemissuccinato de doxilamina	14K27-B07-303356	1
Fagron	Hemissuccinato de doxilamina	15F01-B04-308354	1
Fagron	Hemissuccinato de doxilamina	15F01-B04-309189	3
Fagron	Hemissuccinato de doxilamina	15K04-B01	1
Fagron	Hemissuccinato de doxilamina	15K04-B01-317386	1
Fagron	Hemissuccinato de doxilamina	15K04-B01-318794	5
Fagron	Hemissuccinato de doxilamina	15K04-B01-327356	2
Fagron	Hemissuccinato de doxilamina	15k04b01327357	1
Fagron	Hemissuccinato de doxilamina	16F06-B02	2
Fagron	Hemissuccinato de doxilamina	16F06-B-02-338804	1
Fagron	Hemissuccinato de doxilamina	16F06-B02-338805	4
Fagron	Hemissuccinato de doxilamina	16-F06-B02-338805	1
Fagron	Hemissuccinato de doxilamina	16F06-B02-341879	7
Fagron	Hemissuccinato de doxilamina	16F06-B02-348870	2
Fagron	Hemissuccinato de doxilamina	16F-06-B02-348870	1
Fagron	Hemissuccinato de doxilamina	16F-06-B02-3488760	1
Fagron	Hemissuccinato de doxilamina	16F-06-B02-351516	1
Fagron	Hemissuccinato de doxilamina	16F06-B02-353930	3
Fagron	Hemissuccinato de doxilamina	16F06-B02-353931	5
Fagron	Hemissuccinato de doxilamina	16F06-B02-357510	2
Fagron	Hemissuccinato de doxilamina	16F06-B02-357986	2
Fagron	Hemissuccinato de doxilamina	18041818	1
Fagron	Hemissuccinato de doxilamina	19C14-B01	1
Fagron	Hemissuccinato de doxilamina	19C14-B01-362199	2
Fagron	Hemissuccinato de doxilamina	19C14-B01-362200	2
Fagron	Hemissuccinato de doxilamina	19C14-B01-364554	1
Fagron	Hemissuccinato de doxilamina	19C14-B01-364555	2
Fagron	Hemissuccinato de doxilamina	19C14-B01-364557	1
Fagron	Hemissuccinato de doxilamina	19C14-B01-364888	1
Fagron	Hemissuccinato de doxilamina	20B19-F06-368886	2
Fagron	Hemissuccinato de doxilamina	20B19-F06-370985	2
Fagron	Hemissuccinato de doxilamina	20B19-F06-370986	1
Fagron	Hemissuccinato de doxilamina	20B19-F06-370987	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hemissuccinato de doxilamina	20K05-F03	2
Fagron	Hemissuccinato de doxilamina	21C19-F04-377750	2
Fagron	Hemissuccinato de doxilamina	21C19-F04-377751	1
Fagron	Hemissuccinato de doxilamina	2oko5-F03-375372	1
Fagron	Hemissuccinato de doxilamina	351516	1
Fagron	Hemissuccinato de doxilamina	483875887	1
Fagron	Hemissuccinato de doxilamina	F06-B02-351516/34887	1
L10	Hemissuccinato de doxilamina	16F06B02338805	1
L10	Hemissuccinato de doxilamina	16F06-B02-341879	2
L10	Hemissuccinato de doxilamina	16F06-B02-351516	1
L12	Hemissuccinato de doxilamina	15K04-B01-322165	7
L12	Hemissuccinato de doxilamina	15K04-B01-327357	8
L12	Hemissuccinato de doxilamina	15K04-B01-332765	3
L12	Hemissuccinato de doxilamina	16F06-B02-338805	5
L12	Hemissuccinato de doxilamina	16F06-B02-348870	4
L30	Hemissuccinato de doxilamina	16F06-b02-334258	1
L30	Hemissuccinato de doxilamina	16F06-B02-343936	5

- 235 901 spectra from 1515 *Apo-Ident* customers from a total of 49 184 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hemissuccinato de doxilamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hemissuccinato de doxilamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	300	0	201 784
Type C	0	165	1	235 901

The substance/substance group *Hemissuccinato de doxilamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.3976 % (> 97.5904 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21542	21542	0,00	122,57
22601	22601	0,00	109,97
23085	24535	21,30	107,14
23086	24535	20,16	107,37
24535	24535	0,00	104,46
25518	22601	29,09	107,22
25838	21542	11,81	113,07

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hemissuccinato de prednisolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20838-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hemissuccinato de prednisolona; Prednisolona, hemisuccinato; Prednisoloni hydrogenosuccinas

Special notes

When selecting the *Hemissuccinato de prednisolona* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hemissuccinato de prednisolona	3	2	10

Second-stage model

For differentiation of the substance/substance group *Hemissuccinato de prednisolona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hemissuccinato de prednisolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estriol	80,66	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hemissuccinato de prednisolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hemissuccinato de prednisolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Hemissuccinato de prednisolona	2011003	25644	40	20201223*
Fagron	Hemissuccinato de prednisolona	13D16-N11	20956	40	1509250
Fagron	Hemissuccinato de prednisolona	14G29-B07-304733	22652	40	1701370
Fagron	Hemissuccinato de prednisolona	14G29-B07-304733	22723	40	20140825

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Hemissuccinato de prednisolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 802 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Hemissuccinato de prednisolona*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hemissuccinato de prednisolona	12A20-N11	20838	40
Fagron	Hemissuccinato de prednisolona	15C11-B05-344778	24058	40

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 12 *Apo-Ident* customers from 11 batches from the substance/substance group *Hemissuccinato de prednisolona*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Hemissuccinato de prednisolona	12A20-N11	1
Caelo	Hemissuccinato de prednisolona	14G29-B07	1
Caelo	Hemissuccinato de prednisolona	15C11B05328275	1
Caelo	Hemissuccinato de prednisolona	15C11-B05-305533	1
Caelo	Hemissuccinato de prednisolona	19081502	1
Fagron	Hemissuccinato de prednisolona	12L14-N04	1
Fagron	Hemissuccinato de prednisolona	14G29-B07-304733	1
Fagron	Hemissuccinato de prednisolona	15c11-B05338297	1
Fagron	Hemissuccinato de prednisolona	15C11-B05-338297	2
Fagron	Hemissuccinato de prednisolona	15C11-B05-344778	5
Phönix	Hemissuccinato de prednisolona	13H24-N04	1

- 236 051 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hemissuccinato de prednisolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hemissuccinato de prednisolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	80	0	202 004
Type C	0	16	0	236 051

The substance/substance group *Hemissuccinato de prednisolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20956	20956	0,00	82,86
22652	22652	0,00	80,66
22723	22652	3,20	82,30
25644	25644	0,00	83,41

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hemitartarato de epinefrina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20689-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hemitartarato de epinefrina; Adrenalini tartras; Epinefrina, hemitartarato

Special notes

When selecting the *Hemitartarato de epinefrina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hemitartarato de epinefrina	7	5	34

Second-stage model

For differentiation of the substance/substance group *Hemitartarato de epinefrina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hemitartarato de epinefrina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	100,16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hemitartarato de epinefrina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hemitartarato de epinefrina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hemitartarato de epinefrina	12120202	20689	40	1405614
Caelo	Hemitartarato de epinefrina	12337804	21058	40	20121128
Caelo	Hemitartarato de epinefrina	14007802	21489	60	1603180
Caelo	Hemitartarato de epinefrina	14007802	21489SI	60	1603180
Caelo	Hemitartarato de epinefrina	14007802	21490	60	20140130
Caelo	Hemitartarato de epinefrina	14007802	21491	20	20140130
Caelo	Hemitartarato de epinefrina	14007802	21492	20	20140130
Caelo	Hemitartarato de epinefrina	14007802	21493	20	20140130
Caelo	Hemitartarato de epinefrina	14007802	21494	60	20140130
Caelo	Hemitartarato de epinefrina	14007802	21495	20	20140130
Caelo	Hemitartarato de epinefrina	14007802	21496	20	20140130
Caelo	Hemitartarato de epinefrina	14007802	21497	20	20140130
Caelo	Hemitartarato de epinefrina	14007802	21498	20	20140130
Caelo	Hemitartarato de epinefrina	20004277006	25728	40	20201214
Caelo	Hemitartarato de epinefrina	20004277006	25728SI	40	20201214
Caelo	Hemitartarato de epinefrina	21004241	26299	40	20220622*
Caelo	Hemitartarato de epinefrina	21004241	26299SI	40	20220622*
Fagron	Hemitartarato de epinefrina	12L22-N04	20749	40	20120106
Fagron	Hemitartarato de epinefrina	18K30-B03-358514	24706	40	20190320

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 700 spectra of 19 reference samples from the substance/substance group *Hemitartarato de epinefrina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 262 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 720 spectra of 21 reference samples from the substance/substance group *Hemitartarato de epinefrina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hemitartarato de epinefrina	162764	22777	40
Caelo	Hemitartarato de epinefrina	171115	23323	40
Caelo	Hemitartarato de epinefrina	181795	24260	40
Caelo	Hemitartarato de epinefrina	22002542002	26553	40
Caelo	Hemitartarato de epinefrina	24000754	27466	40
Caelo	Hemitartarato de epinefrina	14007802	21490SI†	60
Caelo	Hemitartarato de epinefrina	14007802	21491SI†	20
Caelo	Hemitartarato de epinefrina	14007802	21492SI†	20
Caelo	Hemitartarato de epinefrina	14007802	21493SI†	20
Caelo	Hemitartarato de epinefrina	14007802	21495SI†	20
Caelo	Hemitartarato de epinefrina	14007802	21496SI†	20
Caelo	Hemitartarato de epinefrina	14007802	21497SI†	20
Caelo	Hemitartarato de epinefrina	14007802	21498SI†	20
Caelo	Hemitartarato de epinefrina	162764	22777SI	40
Caelo	Hemitartarato de epinefrina	171115	23323SI	40
Caelo	Hemitartarato de epinefrina	171115	23326	40
Caelo	Hemitartarato de epinefrina	171115	23326SI	40
Caelo	Hemitartarato de epinefrina	181795	24260SI	40
Caelo	Hemitartarato de epinefrina	22002542002	26553SI	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hemitartarato de epinefrina	24000754	27466SI	40
Fagron	Hemitartarato de epinefrina	18K30-B03-358514	24706SI†	40

- 201 364 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 68 spectra from 37 *Apo-Ident* customers from 38 batches from the substance/substance group *Hemitartarato de epinefrina*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD 17.11.14 EK 7,60	Hemitartarato de epinefrina		1
Alliance Health 12.03.14	Hemitartarato de epinefrina	12337805	1
Caelo	Hemitartarato de epinefrina	10237109	1
Caelo	Hemitartarato de epinefrina	12120202	1
Caelo	Hemitartarato de epinefrina	123337805	1
Caelo	Hemitartarato de epinefrina	12337801	1
Caelo	Hemitartarato de epinefrina	12337805	2
Caelo	Hemitartarato de epinefrina	14007808	1
Caelo	Hemitartarato de epinefrina	14301002	2
Caelo	Hemitartarato de epinefrina	15194102	2
Caelo	Hemitartarato de epinefrina	15194104	1
Caelo	Hemitartarato de epinefrina	15239701	2
Caelo	Hemitartarato de epinefrina	15239703	1
Caelo	Hemitartarato de epinefrina	162746402	1
Caelo	Hemitartarato de epinefrina	16276402	2
Caelo	Hemitartarato de epinefrina	16276406	2
Caelo	Hemitartarato de epinefrina	17111503	3
Caelo	Hemitartarato de epinefrina	181795003	1
Caelo	Hemitartarato de epinefrina	18179503	2
Caelo	Hemitartarato de epinefrina	18179504	5
Caelo	Hemitartarato de epinefrina	18179505	2
Caelo	Hemitartarato de epinefrina	20004277006	1
Caelo	Hemitartarato de epinefrina	210316-1	1
Caelo	Hemitartarato de epinefrina	210316-3	1
Caelo	Hemitartarato de epinefrina	22002542002	2
Caesar & Loretz GmbH...	Hemitartarato de epinefrina	20004277006	1
Caesar & Loretz GmbH	Hemitartarato de epinefrina	18179505	1
Caesar & Loretz GmbH	Hemitartarato de epinefrina	20004277006	2
Caesar & Loretz GmbH	Hemitartarato de epinefrina	22002542002	1
Fagron	Hemitartarato de epinefrina	12/02-N03	1
Fagron	Hemitartarato de epinefrina	12011902	1
Fagron	Hemitartarato de epinefrina	12G11-N07	1
Fagron	Hemitartarato de epinefrina	12G11-No70076/130	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hemitartarato de epinefrina	13I04-N03	1
Fagron	Hemitartarato de epinefrina	13I04-N03	1
Fagron	Hemitartarato de epinefrina	14E12-B02	1
Fagron	Hemitartarato de epinefrina	15A13-B02-305559	2
Fagron	Hemitartarato de epinefrina	16e09-b11-319882	1
Fagron	Hemitartarato de epinefrina	16E09-B11-319882	4
Fagron	Hemitartarato de epinefrina	E80-18002	4
Fagron	Hemitartarato de epinefrina	E80-18D02	1
Gehe	Hemitartarato de epinefrina	17111503	1
GEHE	Hemitartarato de epinefrina	18179504	1
Phoenix 22.5.14	Hemitartarato de epinefrina	12337804	1
Wuhan/Noweda	Hemitartarato de epinefrina	C38-190902	1

- 235 999 spectra from 1515 *Apo-Ident* customers from a total of 49 220 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hemitartarato de epinefrina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hemitartarato de epinefrina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	700	0	152 262
Type B	0	720	0	201 364
Type C	0	68	0	235 999

The substance/substance group *Hemitartarato de epinefrina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1429 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.1765 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20689	20689	0,00	235,16
20749	21489	18,60	230,38
21058	20689	5,20	235,13
21489	21489	0,00	247,01
21490	21489	5,01	258,96
21491	21489	2,92	246,66
21492	21489	6,41	231,24
21493	21489	2,24	244,01
21494	21489	9,45	241,82
21495	21489	3,91	246,94
21496	21489	6,58	234,44
21497	20689	8,79	231,07
21498	21489	2,98	245,77
24706	20689	6,52	238,21
25728	21489	9,09	243,87
26299	26299	0,00	236,42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Heparina sódica**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20638-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Heparina sódica; Heparinum natricum

Special notes

When selecting the *Heparina sódica* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Heparina sódica	7	15	30

Second-stage model

For differentiation of the substance/substance group *Heparina sódica* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Heparina sódica* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	71,34	–
⋮	⋮	⋮
Citrato de sódio	>50	135,15
Capsaicina	>50	277,43
Sacarose	>50	359,22
Cloridrato de oxibutinina	>50	469,38
Prednicarbato	>50	490,13
Cloridrato de quinina di-hidratado	>50	553,80
Levocarnitina	>50	580,85
Piridoxal-5-fosfato	>50	678,78
Amifampridina	>50	859,05
Cloridrato de ciprofloxacina	>50	868,17
Tetracaína	>50	926,66
Alfaestradiol	>50	1031,27
Metoxisaleno	>50	1037,41
Acetato de noretisterona	>50	1254,84
Acetato de ciproterona	>50	1356,99
Triclosan	>50	1693,44
Cloridrato de amitriptilina	>50	2474,83
Valina	>50	3559,80

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Heparina sódica* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Heparina sódica*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Heparina sódica	12050009-03	21294	40	AR-15-FG-007427-02
Euro OTC	Heparina sódica	1605022-01	22804	40	9699

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Heparina sódica	12H30-N07	20798	40	1404230
Fagron	Heparina sódica	12L20-B01-317990	22824	40	20130312
Yino Pharma	Heparina sódica	YN01011170904	23978	40	20180411*
Yino Pharma	Heparina sódica	YN01011170904	23979	40	20180411*
Yino Pharma	Heparina sódica	YN01011170502	23980	40	20180411*
Yino Pharma	Heparina sódica	YN01011170502	23981	40	20180411*
Yino Pharma	Heparina sódica	YN01011170904	24195	40	20180531*
Yino Pharma	Heparina sódica	YN010182005002	25757	50	20200528*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 10 reference samples from the substance/substance group *Heparina sódica*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 552 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 750 spectra of 19 reference samples from the substance/substance group *Heparina sódica*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Heparina sódica	1908030-01	25783	50
Fagron	Heparina sódica	16I26-B02-332108	23591	40
Fagron	Heparina sódica	21E10-B02-220313	26391	40
Fagron	Heparina sódica	22K21-B06-224495	26665	40
Yino Pharma	Heparina sódica	YN01011R1170803	23976	40
Yino Pharma	Heparina sódica	YN010111805002	24196	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Yino Pharma	Heparina sódica	YN010121805010	24197	40
Yino Pharma	Heparina sódica	YN01011R11901002	24907	40
Yino Pharma	Heparina sódica	YN010111906005	24908	40
Yino Pharma	Heparina sódica	YN010111906006	24909	40
Yino Pharma	Heparina sódica	YN010111907007	24910	40
Yino Pharma	Heparina sódica	YN010111908008	24911	40
Yino Pharma	Heparina sódica	YN010121810018	24912	40
Yino Pharma	Heparina sódica	YN010111910009	24984	40
Yino Pharma	Heparina sódica	YN010112107004	25758	50
Fagron	Heparina sódica	21E10-B02-220313	26391SI	20
Fagron	Heparina sódica	22K21-B06-224495	26665SI	20
Yino Pharma	Heparina sódica	YN01011R1170803	23977	40
Yino Pharma	Heparina sódica	YN01011R11901002	25756	50

- 201 334 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 45 spectra from 24 *Apo-Ident* customers from 31 batches from the substance/substance group *Heparina sódica*.
- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Heparina sódica	20K06-B02-200814	1
	Heparina sódica	21E10-B02-220313	4
Caelo	Heparina sódica	13G03-N13	2
Caelo	Heparina sódica	16I26-B02-327885	1
Changzhou Qianhong B...	Heparina sódica	20K06-B02-200814	1
Euro OTC	Heparina sódica	1605022-02	2
Fagron	Heparina sódica	11190188SH	2
Fagron	Heparina sódica	12190453CQ	1
Fagron	Heparina sódica	12G19-B02-313422	1
Fagron	Heparina sódica	12H30-N07	2
Fagron	Heparina sódica	12I20-B01-323107	1
Fagron	Heparina sódica	13G03-N13	1
Fagron	Heparina sódica	14D09-B08-293944	2
Fagron	Heparina sódica	14D09-B08-307077	1
Fagron	Heparina sódica	15A20-B02-307307	1
Fagron	Heparina sódica	16I26-B02	1
Fagron	Heparina sódica	16I26-B02-327885	1
Fagron	Heparina sódica	16I26-B02-332108	1
Fagron	Heparina sódica	16I26-B02-342640	1
Fagron	Heparina sódica	17L06-B01	1
Fagron	Heparina sódica	17L06-B01-354811	1
Fagron	Heparina sódica	18C21-B03-349501	1
Fagron	Heparina sódica	19J11B02195123	1
Fagron	Heparina sódica	20D28-B01	2
Fagron	Heparina sódica	20D28-B01-201583	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Heparina sódica	20K06-B02-200814	1
Fagron	Heparina sódica	21E10-B02-213670	2
Fagron	Heparina sódica	B01-2015803	1
Fagron	Heparina sódica	B02-1951203	1
Faron/Kehr /07.07.2020	Heparina sódica	19J11-B02-195122	1
Fiebig	Heparina sódica	16190116C0	1
Gatt-Koller	Heparina sódica	1901027	1
L31	Heparina sódica	16I26-B02-337593	1
Phoenix	Heparina sódica	5920101900	1

- 236 022 spectra from 1515 *Apo-Ident* customers from a total of 49 227 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Heparina sódica* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Heparina sódica* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	750	0	201 334
Type C	0	44	1	236 022

The substance/substance group *Heparina sódica* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2000 %)
Type C	100.0000 % (> 99.9007 %)	97.7778 % (> 91.1111 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20798	20798	0,00	112,89
21294	21294	0,00	76,55
22804	22804	0,00	69,95
22824	21294	19,65	99,98
23978	23978	0,00	50,38
23979	23979	0,00	51,39
23980	23980	0,00	63,70
23981	23981	0,00	76,07
24195	24195	0,00	86,76
25757	25757	0,00	93,52

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hiclato de doxiciclina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20796-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hiclato de doxiciclina; Doxiciclina, hiclato; Doxycyclini hyclas

Special notes

When selecting the *Hiclato de doxiciclina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hiclato de doxiciclina	6	3	31

Second-stage model

For differentiation of the substance/substance group *Hiclato de doxiciclina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hiclato de doxiciclina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	74,46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hiclato de doxiciclina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hiclato de doxiciclina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hiclato de doxiciclina	12G12-N15	20796	40	1404233
Fagron	Hiclato de doxiciclina	12G12-N15	20821	40	20120807
Fagron	Hiclato de doxiciclina	14K28-B05-312218	22242	60	20150216
Fagron	Hiclato de doxiciclina	19A30-B01-360207	24820	40	20190412
Fagron	Hiclato de doxiciclina	19I12-F01-366406	24946	40	20191204
Fagron	Hiclato de doxiciclina	21I10-B02-219301	26328	40	20211117
Fagron	Hiclato de doxiciclina	21I10-B02-219301	26328SI	20	20211117
Fagron	Hiclato de doxiciclina	23L01-B01-004244	27469	40	20231219

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 8 reference samples from the substance/substance group *Hiclato de doxiciclina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Hiclato de doxiciclina*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hiclato de doxiciclina	16I06-B02-330167	23118	40
Fagron	Hiclato de doxiciclina	18D18-B01-349567	24170	40
Fagron	Hiclato de doxiciclina	21I15-F01-380126	25905	40
Fagron	Hiclato de doxiciclina	21I15-F01-380126	25905SI	10
Fagron	Hiclato de doxiciclina	23L01-B01-004244	27469SI†	20

- 201 934 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 40 spectra from 27 *Apo-Ident* customers from 33 batches from the substance/substance group *Hiclato de doxiciclina*.
- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hiclato de doxiciclina	2115-F01-380126	1
	Hiclato de doxiciclina	21I10-B02-221825	1
	Hiclato de doxiciclina	H202106006	1
AHD	Hiclato de doxiciclina	18D18-B01-353701	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hiclato de doxiciclina	16I06-B02-335675	1
Caelo	Hiclato de doxiciclina	16I06-B02-341857	1
Fagron	Hiclato de doxiciclina	12G12-N15	1
Fagron	Hiclato de doxiciclina	13D24-B40-298948	1
Fagron	Hiclato de doxiciclina	14K28-B05_312218	1
Fagron	Hiclato de doxiciclina	14K28-B05-312010	1
Fagron	Hiclato de doxiciclina	16/06-B02-341857	1
Fagron	Hiclato de doxiciclina	1603008	1
Fagron	Hiclato de doxiciclina	1606B02330167	1
Fagron	Hiclato de doxiciclina	16106-Bo2	1
Fagron	Hiclato de doxiciclina	16E04-B07-231917	1
Fagron	Hiclato de doxiciclina	16I06-B02	1
Fagron	Hiclato de doxiciclina	16I06-B02-330167	1
Fagron	Hiclato de doxiciclina	16I06-B02-341857	4
Fagron	Hiclato de doxiciclina	16l06-B02-330167	1
Fagron	Hiclato de doxiciclina	17112201	1
Fagron	Hiclato de doxiciclina	18D18_B01_349567	1
Fagron	Hiclato de doxiciclina	18D18-B01-349567	2
Fagron	Hiclato de doxiciclina	18D18B01353701	1
Fagron	Hiclato de doxiciclina	18D18-B01-353701	1
Fagron	Hiclato de doxiciclina	18D18-B01-353801	1
Fagron	Hiclato de doxiciclina	19A30-B01	1
Fagron	Hiclato de doxiciclina	19A30-B01-360207	1
Fagron	Hiclato de doxiciclina	20101701	1
Fagron	Hiclato de doxiciclina	20A30-F01-368711	1
Fagron	Hiclato de doxiciclina	21/10-B02-221825	1
Fagron	Hiclato de doxiciclina	F01-3687101	1
Fragron/Sanacorp	Hiclato de doxiciclina	16l06-B02-335675	1
Löwen City-Apotheke …	Hiclato de doxiciclina	10022014	1
Löwen City-Apotheke …	Hiclato de doxiciclina	2042015	1
Merck	Hiclato de doxiciclina	22022019	1
Sanacorp	Hiclato de doxiciclina	16I06-B02-335675	1

- 236 027 spectra from 1515 *Apo-Ident* customers from a total of 49 226 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hiclato de doxiciclina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hiclato de doxiciclina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	150	0	201 934
Type C	0	39	1	236 027

The substance/substance group *Hiclato de doxiciclina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	97.5000 % (> 90.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20796	20796	0,00	154,38
20821	20796	9,22	153,01
22242	20796	21,48	154,76
24820	20796	19,13	158,01
24946	20796	17,64	162,00
26328	20796	22,67	154,93
27469	20796	12,71	157,72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidrato de cloral**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20322-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidrato de cloral; Chlorali hydras

Special notes

When selecting the *Hidrato de cloral* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidrato de cloral	6	11	189

Second-stage model

For differentiation of the substance/substance group *Hidrato de cloral* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidrato de cloral* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	91,99	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidrato de cloral* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidrato de cloral*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidrato de cloral	13213311	21309	40	20130712
Caelo	Hidrato de cloral	15448318	22963	40	1704462
Caelo	Hidrato de cloral	16355802	23094	40	20170112
Fagron	Hidrato de cloral	13F06-N07	21231	40	20130626
Fagron	Hidrato de cloral	17E05-B05-335580	23572	40	20170623
Fagron	Hidrato de cloral	19K04-B01-201434	25488	40	20191128

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Hidrato de cloral*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 722 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 530 spectra of 14 reference samples from the substance/substance group *Hidrato de cloral*.
- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidrato de cloral	154483	23355	40
Caelo	Hidrato de cloral	172506	23646	40
Caelo	Hidrato de cloral	172477	23678	40
Caelo	Hidrato de cloral	190914	24556	40
Caelo	Hidrato de cloral	192361	24882	40
Caelo	Hidrato de cloral	192872	24891	40
Caelo	Hidrato de cloral	21001025	25668	50
Caelo	Hidrato de cloral	22004038	26689	40
Caelo	Hidrato de cloral	24001050	27304	40
Fagron	Hidrato de cloral	22D25-B01-220429	26180	40
Fagron	Hidrato de cloral	24A24-B10-238074	27185	40
Caelo	Hidrato de cloral	172477	23815	40
Caelo	Hidrato de cloral	22004038	26689SI	20
Fagron	Hidrato de cloral	22D25-B01-220429	26180SI	20

- 201 554 spectra from a total of 4034 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1091 spectra from 423 *Apo-Ident* customers from 195 batches from the substance/substance group *Hidrato de cloral*.
- Among them are spectra of independent samples from 189 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hidrato de cloral	10224/2311B066	1
	Hidrato de cloral	21001025007	1
	Hidrato de cloral	21001025014	1
	Hidrato de cloral	21001025019	1
	Hidrato de cloral	21001025020	3
	Hidrato de cloral	21001025024	2
	Hidrato de cloral	22004038001	12
	Hidrato de cloral	22004038003	1
	Hidrato de cloral	22004038004	5
	Hidrato de cloral	22004038007	3
	Hidrato de cloral	2204038001	1
	Hidrato de cloral	24002447003	1
	Hidrato de cloral	24A24-B10-001840	1
	Hidrato de cloral	24A24-B10-229467	2
	Hidrato de cloral	B08-0018309	1
AHD	Hidrato de cloral	22004038001	1
Anzag	Hidrato de cloral	20003841003	1
Apotheke Tellingstedt	Hidrato de cloral	19091404	1
Bombastus	Hidrato de cloral	17346301	1
Caelo	Hidrato de cloral		1
Caelo	Hidrato de cloral	1(2002323002)	1
Caelo	Hidrato de cloral	12017503	1
Caelo	Hidrato de cloral	12017512	1
Caelo	Hidrato de cloral	12017518	1
Caelo	Hidrato de cloral	13002425	2
Caelo	Hidrato de cloral	13213311	1
Caelo	Hidrato de cloral	13d22-n11	1
Caelo	Hidrato de cloral	1403815	1
Caelo	Hidrato de cloral	14038301	2
Caelo	Hidrato de cloral	14038306	1
Caelo	Hidrato de cloral	14038311	5
Caelo	Hidrato de cloral	14101307	1
Caelo	Hidrato de cloral	14218701	1
Caelo	Hidrato de cloral	14218704	3
Caelo	Hidrato de cloral	14218705	3
Caelo	Hidrato de cloral	14218709	5
Caelo	Hidrato de cloral	14218710	1
Caelo	Hidrato de cloral	14218711	1
Caelo	Hidrato de cloral	14218712	1
Caelo	Hidrato de cloral	14218713	2
Caelo	Hidrato de cloral	14218714	4
Caelo	Hidrato de cloral	14218719	4
Caelo	Hidrato de cloral	14218720	1
Caelo	Hidrato de cloral	15083701	2
Caelo	Hidrato de cloral	15083703	8
Caelo	Hidrato de cloral	15083704	1
Caelo	Hidrato de cloral	15083705	2
Caelo	Hidrato de cloral	15163901	1
Caelo	Hidrato de cloral	15166501	4
Caelo	Hidrato de cloral	15166502	3
Caelo	Hidrato de cloral	15166503	4
Caelo	Hidrato de cloral	15166505	11
Caelo	Hidrato de cloral	15166506	7
Caelo	Hidrato de cloral	15166507	10
Caelo	Hidrato de cloral	15166508	6
Caelo	Hidrato de cloral	15166513	3
Caelo	Hidrato de cloral	15448303	3
Caelo	Hidrato de cloral	15448304	2
Caelo	Hidrato de cloral	15448306	7
Caelo	Hidrato de cloral	15448307	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrato de cloral	15448310	1
Caelo	Hidrato de cloral	15448312	11
Caelo	Hidrato de cloral	15448313	8
Caelo	Hidrato de cloral	15448314	6
Caelo	Hidrato de cloral	15448315	6
Caelo	Hidrato de cloral	15448318	10
Caelo	Hidrato de cloral	15448320	6
Caelo	Hidrato de cloral	15448321	7
Caelo	Hidrato de cloral	15448322	7
Caelo	Hidrato de cloral	15448324	10
Caelo	Hidrato de cloral	15448325	2
Caelo	Hidrato de cloral	15448326	10
Caelo	Hidrato de cloral	15448327	1
Caelo	Hidrato de cloral	15458322	1
Caelo	Hidrato de cloral	160906C	1
Caelo	Hidrato de cloral	16248703	1
Caelo	Hidrato de cloral	16355803	1
Caelo	Hidrato de cloral	16355804	2
Caelo	Hidrato de cloral	16355810	1
Caelo	Hidrato de cloral	16355811	2
Caelo	Hidrato de cloral	17121402	1
Caelo	Hidrato de cloral	17247702	20
Caelo	Hidrato de cloral	17247704	16
Caelo	Hidrato de cloral	17250601	14
Caelo	Hidrato de cloral	17314301	3
Caelo	Hidrato de cloral	17314303	1
Caelo	Hidrato de cloral	17314309	1
Caelo	Hidrato de cloral	17314312	1
Caelo	Hidrato de cloral	17314318	2
Caelo	Hidrato de cloral	17314319	1
Caelo	Hidrato de cloral	17314320	1
Caelo	Hidrato de cloral	17314322	5
Caelo	Hidrato de cloral	173406306	1
Caelo	Hidrato de cloral	1734602	1
Caelo	Hidrato de cloral	17346301	28
Caelo	Hidrato de cloral	17346302	16
Caelo	Hidrato de cloral	173463021	1
Caelo	Hidrato de cloral	17346303	5
Caelo	Hidrato de cloral	17346306	45
Caelo	Hidrato de cloral	17346307	21
Caelo	Hidrato de cloral	17346308	14
Caelo	Hidrato de cloral	17346309	11
Caelo	Hidrato de cloral	17346310	12
Caelo	Hidrato de cloral	17346311	10
Caelo	Hidrato de cloral	1746302	1
Caelo	Hidrato de cloral	17520601	1
Caelo	Hidrato de cloral	17550601	1
Caelo	Hidrato de cloral	18054001	1
Caelo	Hidrato de cloral	18327909	1
Caelo	Hidrato de cloral	19000511001	14
Caelo	Hidrato de cloral	19000511003	5
Caelo	Hidrato de cloral	19091401	6
Caelo	Hidrato de cloral	19091402	1
Caelo	Hidrato de cloral	19091404	5
Caelo	Hidrato de cloral	19091405	4
Caelo	Hidrato de cloral	19091408	4
Caelo	Hidrato de cloral	19091409	3
Caelo	Hidrato de cloral	19091410	3
Caelo	Hidrato de cloral	19236101	12
Caelo	Hidrato de cloral	19236102	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrato de cloral	19236103	2
Caelo	Hidrato de cloral	19236104	3
Caelo	Hidrato de cloral	192872001	37
Caelo	Hidrato de cloral	192872002	3
Caelo	Hidrato de cloral	192872003	4
Caelo	Hidrato de cloral	192872004	3
Caelo	Hidrato de cloral	19287201	8
Caelo	Hidrato de cloral	19287206	5
Caelo	Hidrato de cloral	200002323002	1
Caelo	Hidrato de cloral	20002323002	35
Caelo	Hidrato de cloral	20002323004	6
Caelo	Hidrato de cloral	2000233002	1
Caelo	Hidrato de cloral	20003841002	11
Caelo	Hidrato de cloral	20003841003	42
Caelo	Hidrato de cloral	20003841005	2
Caelo	Hidrato de cloral	2003841003	1
Caelo	Hidrato de cloral	2019Q-01257	1
Caelo	Hidrato de cloral	21001025002	6
Caelo	Hidrato de cloral	21001025003	4
Caelo	Hidrato de cloral	21001025004	29
Caelo	Hidrato de cloral	21001025005	19
Caelo	Hidrato de cloral	21001025007	4
Caelo	Hidrato de cloral	21001025009	1
Caelo	Hidrato de cloral	21001025010	15
Caelo	Hidrato de cloral	21001025014	1
Caelo	Hidrato de cloral	21001025015	5
Caelo	Hidrato de cloral	21001025016	1
Caelo	Hidrato de cloral	21001025017	4
Caelo	Hidrato de cloral	21001025019	1
Caelo	Hidrato de cloral	21001025020	1
Caelo	Hidrato de cloral	21001025023	1
Caelo	Hidrato de cloral	210010250236	2
Caelo	Hidrato de cloral	21001025024	6
Caelo	Hidrato de cloral	2100105004	1
Caelo	Hidrato de cloral	22004038001	1
Caelo	Hidrato de cloral	25021401	1
Caelo	Hidrato de cloral	2818A-01257	1
Caelo	Hidrato de cloral	2826	1
Caelo	Hidrato de cloral	30081807	1
Caelo	Hidrato de cloral	3121403	1
Caelo	Hidrato de cloral	3299	1
Caelo	Hidrato de cloral	3333	1
Caelo	Hidrato de cloral	3449	1
Caelo	Hidrato de cloral	4616Q-01257	1
Caelo	Hidrato de cloral	6051703	1
Caelo	Hidrato de cloral	928720011	1
Caeol/Noweda	Hidrato de cloral	15448313	1
Caesar & Lorenz GmbH	Hidrato de cloral	19000511001	1
Caesar & Lorenz GmbH	Hidrato de cloral	192872001	1
Caesar & Loretz GmbH…	Hidrato de cloral	20003841003	1
Caesar & Loretz GmbH…	Hidrato de cloral	21001025004	1
Caesar & Loretz GmbH…	Hidrato de cloral	21001025004	1
Caesar & Loretz GmbH…	Hidrato de cloral	21001025005	1
Caesar & Loretz GmbH…	Hidrato de cloral	20003841003	1
Caesar & Loretz GmbH…	Hidrato de cloral	20003841003	2
Caesar & Loretz GmbH…	Hidrato de cloral	119236101	1
Caesar & Loretz GmbH…	Hidrato de cloral	20002323002	1
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	19000511001	1
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	19236101	1
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	20002323002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	20003841003	1
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	21001025005	1
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	21001025020	3
Caesar & Loretz GmbH/Gehe	Hidrato de cloral	21001025024	1
Caesar & Loretz GmbH...	Hidrato de cloral	20002323003	2
Caesar & Loretz GmbH...	Hidrato de cloral	19287206	1
Caesar & Loretz GmbH...	Hidrato de cloral	20002323002	2
Caesar & Loretz GmbH...	Hidrato de cloral	20003841003	1
Caesar & Loretz GmbH...	Hidrato de cloral	21001025010	1
Caesar & Loretz GmbH...	Hidrato de cloral	21001025016	1
Caesar & Loretz GmbH...	Hidrato de cloral	21001025024	2
Caesar & Loretz GmbH...	Hidrato de cloral	22004038001	4
Caesar & Loretz GmbH...	Hidrato de cloral	192872001	1
Caesar & Loretz GmbH...	Hidrato de cloral	21001025010	1
Caesar & Loretz GmbH...	Hidrato de cloral	21001025024	1
Caesar & Loretz GmbH	Hidrato de cloral	17314317	1
Caesar & Loretz GmbH	Hidrato de cloral	17314319	2
Caesar & Loretz GmbH	Hidrato de cloral	17314320	1
Caesar & Loretz GmbH	Hidrato de cloral	17346301	1
Caesar & Loretz GmbH	Hidrato de cloral	17346310	1
Caesar & Loretz GmbH	Hidrato de cloral	19000511001	1
Caesar & Loretz GmbH	Hidrato de cloral	19091401	1
Caesar & Loretz GmbH	Hidrato de cloral	19091409	2
Caesar & Loretz GmbH	Hidrato de cloral	19236101	1
Caesar & Loretz GmbH	Hidrato de cloral	19236104	1
Caesar & Loretz GmbH	Hidrato de cloral	192872001	6
Caesar & Loretz GmbH	Hidrato de cloral	192872002	1
Caesar & Loretz GmbH	Hidrato de cloral	192872004	3
Caesar & Loretz GmbH	Hidrato de cloral	19287201	1
Caesar & Loretz GmbH	Hidrato de cloral	19287206	1
Caesar & Loretz GmbH	Hidrato de cloral	20002323002	11
Caesar & Loretz GmbH	Hidrato de cloral	20002323004	6
Caesar & Loretz GmbH	Hidrato de cloral	20002323022	1
Caesar & Loretz GmbH	Hidrato de cloral	20003841002	6
Caesar & Loretz GmbH	Hidrato de cloral	20003841003	13
Caesar & Loretz GmbH	Hidrato de cloral	20003841004	2
Caesar & Loretz GmbH	Hidrato de cloral	20003841005	3
Caesar & Loretz GmbH	Hidrato de cloral	21001025002	2
Caesar & Loretz GmbH	Hidrato de cloral	21001025003	1
Caesar & Loretz GmbH	Hidrato de cloral	21001025004	5
Caesar & Loretz GmbH	Hidrato de cloral	21001025005	3
Caesar & Loretz GmbH	Hidrato de cloral	21001025007	1
Caesar & Loretz GmbH	Hidrato de cloral	21001025009	2
Caesar & Loretz GmbH	Hidrato de cloral	21001025010	10
Caesar & Loretz GmbH	Hidrato de cloral	21001025012	2
Caesar & Loretz GmbH	Hidrato de cloral	21001025016	3
Caesar & Loretz GmbH	Hidrato de cloral	21001025017	1
Caesar & Loretz GmbH	Hidrato de cloral	21001025024	1
Caesar & Loretz GmbH	Hidrato de cloral	21001025026	1
Caesar & Loretz Hild...	Hidrato de cloral	192872001	1
Caesar & Loretz/AHD	Hidrato de cloral	20002323002	1
Caesar & Loretz/Noweda	Hidrato de cloral	20003841003	1
Caesar/Phoenix	Hidrato de cloral	17250601	1
Caesar	Hidrato de cloral	15166501	1
Cealo/ Alliance	Hidrato de cloral	17247702	1
chaelo/gehe	Hidrato de cloral	20003841003	3
Chemische Fabrik Ber...	Hidrato de cloral	192872001	2
Ebert & Jacobi	Hidrato de cloral	16D14-B02-322991	1
Ebert KKH 10.10.16	Hidrato de cloral	15448308	1
Eder Apotheke	Hidrato de cloral	19236101	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Hidrato de cloral	15448318	1
Euro OTC	Hidrato de cloral	16122001	1
Fagron	Hidrato de cloral	11D13-N07	1
Fagron	Hidrato de cloral	11J05-N01	1
Fagron	Hidrato de cloral	12C26-M04	1
Fagron	Hidrato de cloral	12C26-M05	1
Fagron	Hidrato de cloral	12H06_N08	1
Fagron	Hidrato de cloral	12H06N08	2
Fagron	Hidrato de cloral	12H06-N08	6
Fagron	Hidrato de cloral	12H06-N080101/1612	1
Fagron	Hidrato de cloral	12H06-N080160/161	1
Fagron	Hidrato de cloral	12H06N8	1
Fagron	Hidrato de cloral	13D22-N11	1
Fagron	Hidrato de cloral	13F06-N07	2
Fagron	Hidrato de cloral	13F06-N070631/786	1
Fagron	Hidrato de cloral	13K05-B13	1
Fagron	Hidrato de cloral	14218710	1
Fagron	Hidrato de cloral	14218712	1
Fagron	Hidrato de cloral	15166505	1
Fagron	Hidrato de cloral	160609/1	1
Fagron	Hidrato de cloral	17346301	1
Fagron	Hidrato de cloral	17J31-B02-342155	2
Fagron	Hidrato de cloral	18F15-B01-355393	2
Fagron	Hidrato de cloral	18F15-B01-355394	2
Fagron	Hidrato de cloral	18L18-B01-193679	1
Fagron	Hidrato de cloral	192872002	1
Fagron	Hidrato de cloral	19K04-B01	1
Fagron	Hidrato de cloral	19K04-B01-1955569	1
Fagron	Hidrato de cloral	19K04-B01-195569	1
Fagron	Hidrato de cloral	19K04-B01-201434	3
Fagron	Hidrato de cloral	21001025016	1
Fagron	Hidrato de cloral	21B25-B03-203396	2
Gehe amax	Hidrato de cloral	19000511001	1
Gehe	Hidrato de cloral	15083703	1
GEHE	Hidrato de cloral	15448312	1
Gehe	Hidrato de cloral	15448326	1
Gehe	Hidrato de cloral	17247704	2
Gehe	Hidrato de cloral	17346301	1
Gehe	Hidrato de cloral	192872001	1
Gehe	Hidrato de cloral	2000232302	1
Gehe	Hidrato de cloral	22004038001	1
Gehe	Hidrato de cloral	24002447005	1
Ichthyol GmBH	Hidrato de cloral	13002425	2
Ichthyol	Hidrato de cloral	15448314	1
Jenne	Hidrato de cloral	21001025020	1
Kehr	Hidrato de cloral	17346302	1
Kehr	Hidrato de cloral	22004038001	2
L12	Hidrato de cloral	17346301	1
Noweda	Hidrato de cloral	17314319	1
Noweda	Hidrato de cloral	17346306	1
Noweda	Hidrato de cloral	17346310	1
Noweda	Hidrato de cloral	19091404	1
Noweda	Hidrato de cloral	19091408	1
Noweda	Hidrato de cloral	19287201	1
Noweda	Hidrato de cloral	22004038001	1
Noweda29.04.2015	Hidrato de cloral	15083701	2
Phoenix	Hidrato de cloral	15448318	1
Phoenix	Hidrato de cloral	3187	1
Phönix Gotha	Hidrato de cloral	13F06-N07	2
Phönix Gotha	Hidrato de cloral	14038302	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Hidrato de cloral	17346301	1
Phönix	Hidrato de cloral	17346303	3
Phönix	Hidrato de cloral	17346311	5
Phönix	Hidrato de cloral	192872001	1
Phönix	Hidrato de cloral	22004038001	2
Phönix	Hidrato de cloral	2202204038007	1
Sanacorp	Hidrato de cloral	12H06-N08	3
Sanacorp	Hidrato de cloral	14218705	1
Sanacorp	Hidrato de cloral	15448326	1
Sanacorp	Hidrato de cloral	17346301	1
Sanacorp	Hidrato de cloral	17346306	1
Sanacorp	Hidrato de cloral	192872001	1
Sanacorp	Hidrato de cloral	21001025002	2
Sanacorp	Hidrato de cloral	21001025007	1
Sanacorp	Hidrato de cloral	21001025023	3
Sanacorp	Hidrato de cloral	22004038001	2
Sanacorp	Hidrato de cloral	22004038007	1

- 234 976 spectra from 1515 *Apo-Ident* customers from a total of 49 064 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hidrato de cloral* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidrato de cloral* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	530	0	201 554
Type C	0	1063	28	234 976

The substance/substance group *Hidrato de cloral* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8679 %)
Type C	100.0000 % (> 99.9007 %)	97.4335 % (> 97.1586 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21231	22963	13,12	153,80
21309	22963	6,67	154,57
22963	22963	0,00	148,74
23094	22963	7,61	153,47
23572	22963	5,55	151,56
25488	22963	11,12	156,00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidrocarbonato de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20193-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidrocarbonato de potássio; Kalii hydrogencarbonas

Special notes

When selecting the *Hidrocarbonato de potássio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidrocarbonato de potássio	6	2	47

Second-stage model

For differentiation of the substance/substance group *Hidrocarbonato de potássio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidrocarbonato de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	61,33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidrocarbonato de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidrocarbonato de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidrocarbonato de potássio	23003573	27101	40	20240119*
Euro OTC	Hidrocarbonato de potássio	1805027-01	24271	40	20180606
Euro OTC	Hidrocarbonato de potássio	2204004	26563	40	20220520*
Euro OTC	Hidrocarbonato de potássio	2208022	26564	40	20220902*
Euro OTC	Hidrocarbonato de potássio	2208022	26564SI	20	20220902*
Euro OTC	Hidrocarbonato de potássio	2303001	26637	40	20230314*
Euro OTC	Hidrocarbonato de potássio	2401021	27165	40	20240227*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Hidrocarbonato de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 130 spectra of 4 reference samples from the substance/substance group *Hidrocarbonato de potássio*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Hidrocarbonato de potássio	2107027	25791	50
Euro OTC	Hidrocarbonato de potássio	2408009	27454	40
Euro OTC	Hidrocarbonato de potássio	2204004	26563SI†	20
Euro OTC	Hidrocarbonato de potássio	2303001	26637SI†	20

- 201 954 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 83 spectra from 51 *Apo-Ident* customers from 48 batches from the substance/substance group *Hidrocarbonato de potássio*.

- Among them are spectra of independent samples from 47 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Hidrocarbonato de potássio	21004124012	1
	Hidrocarbonato de potássio	23003573002	1
	Hidrocarbonato de potássio	2303001-01	1
	Hidrocarbonato de potássio	2401021-01	1
Caelo	Hidrocarbonato de potássio		1
Caelo	Hidrocarbonato de potássio	10052610	1
Caelo	Hidrocarbonato de potássio	10052622	1
Caelo	Hidrocarbonato de potássio	10052629	1
Caelo	Hidrocarbonato de potássio	1011M-01728	1
Caelo	Hidrocarbonato de potássio	11105804	1
Caelo	Hidrocarbonato de potássio	11105808	1
Caelo	Hidrocarbonato de potássio	11105811	3
Caelo	Hidrocarbonato de potássio	11105812	1
Caelo	Hidrocarbonato de potássio	11105818	1
Caelo	Hidrocarbonato de potássio	11105822	1
Caelo	Hidrocarbonato de potássio	1214190	1
Caelo	Hidrocarbonato de potássio	12141905	3
Caelo	Hidrocarbonato de potássio	12141910	8
Caelo	Hidrocarbonato de potássio	12141912	3
Caelo	Hidrocarbonato de potássio	12141915	3
Caelo	Hidrocarbonato de potássio	12141919	5
Caelo	Hidrocarbonato de potássio	12141920	1
Caelo	Hidrocarbonato de potássio	12141924	3
Caelo	Hidrocarbonato de potássio	12141930	2
Caelo	Hidrocarbonato de potássio	1214924	1
Caelo	Hidrocarbonato de potássio	12239701	3
Caelo	Hidrocarbonato de potássio	12239702	2
Caelo	Hidrocarbonato de potássio	12239703	3
Caelo	Hidrocarbonato de potássio	1303002-01	1
Caelo	Hidrocarbonato de potássio	13141926	1
Caelo	Hidrocarbonato de potássio	13390303	1
Caelo	Hidrocarbonato de potássio	13390307	1
Caelo	Hidrocarbonato de potássio	20080410-3	1
Caelo	Hidrocarbonato de potássio	24051301	1
Caelo	Hidrocarbonato de potássio	3812Q-01728	1
Caelo	Hidrocarbonato de potássio	6011405	1
Caelo	Hidrocarbonato de potássio	700544	1
Caelo	Hidrocarbonato de potássio	8101202	1
Euro OTC	Hidrocarbonato de potássio	1202013-01	1
Euro OTC	Hidrocarbonato de potássio	1204038-01	1
Euro OTC	Hidrocarbonato de potássio	1208010-01	3
Euro OTC	Hidrocarbonato de potássio	1303002-01	3
Euro OTC	Hidrocarbonato de potássio	2809033-01	1
Euro OTC	Hidrocarbonato de potássio	4413I1728	1
Fagron	Hidrocarbonato de potássio	120801001	1
Fagron	Hidrocarbonato de potássio	12141911	1
Fagron	Hidrocarbonato de potássio	12K27-N06	1
Fagron	Hidrocarbonato de potássio	1303120S	1
holdermann euro	Hidrocarbonato de potássio	1303002-01	1
Noweda	Hidrocarbonato de potássio	1004019-01	1
Phoenix	Hidrocarbonato de potássio	12141915	1
Stumpf	Hidrocarbonato de potássio	1204038-01	1

- 235 984 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Hidrocarbonato de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidrocarbonato de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	130	0	201 954
Type C	0	81	2	235 984

The substance/substance group *Hidrocarbonato de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.9007 %)	97.5904 % (> 93.9759 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24271	27101	9,84	72,13
26563	26563	0,00	73,20
26564	26564	0,00	74,60
26637	26637	0,00	75,07
27101	27101	0,00	73,13
27165	27165	0,00	73,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidroclorotiazida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20323-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidroclorotiazida; Hydrochlorothiazidum

Special notes

When selecting the *Hidroclorotiazida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidroclorotiazida	6	4	111

Second-stage model

For differentiation of the substance/substance group *Hidroclorotiazida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidroclorotiazida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	113,22	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidroclorotiazida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidroclorotiazida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidroclorotiazida	13008505	21589	60	AR-15-FG-014461-01
Caelo	Hidroclorotiazida	182649	24362	40	20181127*
Fagron	Hidroclorotiazida	11L01-N02	20888	40	20111209
Fagron	Hidroclorotiazida	17L20-B02-345079	23989	40	20180125
Fagron	Hidroclorotiazida	20E27-F01-371506	25590	40	20200630
Fagron	Hidroclorotiazida	21H27-B04-220130	26172	40	20220202

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Hidroclorotiazida*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Hidroclorotiazida*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidroclorotiazida	14009701	23116	40
Caelo	Hidroclorotiazida	192328	24888	40
Caelo	Hidroclorotiazida	23002418	27125	40
Fagron	Hidroclorotiazida	16F17-B07-327489	23600	40
Caelo	Hidroclorotiazida	23002418	27125SI	20
Fagron	Hidroclorotiazida	21H27-B04-220130	26172SI†	20

- 201 884 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 440 spectra from 264 *Apo-Ident* customers from 120 batches from the substance/substance group *Hidroclorotiazida*.
- Among them are spectra of independent samples from 110 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Hidroclorotiazida	18017305	1
	Hidroclorotiazida	20004000011	1
	Hidroclorotiazida	20004000014	1
	Hidroclorotiazida	22044HC10RII	1
	Hidroclorotiazida	22K29-B01-224324	3
	Hidroclorotiazida	23002418002	1
	Hidroclorotiazida	23A04-B06-229298	3
	Hidroclorotiazida	23L28-B02-237422	1
	Hidroclorotiazida	B06-2336203	1
AHD	Hidroclorotiazida	17H28-B01-340561	1
Caelo	Hidroclorotiazida	11101n02	1
Caelo	Hidroclorotiazida	13008507	2
Caelo	Hidroclorotiazida	13008509	5
Caelo	Hidroclorotiazida	14009701	25
Caelo	Hidroclorotiazida	140097012	1
Caelo	Hidroclorotiazida	14B10-B01-305043	2
Caelo	Hidroclorotiazida	15231002	3
Caelo	Hidroclorotiazida	15231003	5
Caelo	Hidroclorotiazida	15231005	1
Caelo	Hidroclorotiazida	15231008	2
Caelo	Hidroclorotiazida	15231009	3
Caelo	Hidroclorotiazida	15231011	1
Caelo	Hidroclorotiazida	16269301	4
Caelo	Hidroclorotiazida	16269304	2
Caelo	Hidroclorotiazida	16269306	1
Caelo	Hidroclorotiazida	16269307	3
Caelo	Hidroclorotiazida	16269309	6
Caelo	Hidroclorotiazida	16269311	3
Caelo	Hidroclorotiazida	16269312	2
Caelo	Hidroclorotiazida	16269313	4
Caelo	Hidroclorotiazida	16F17-B07-324062	1
Caelo	Hidroclorotiazida	16F17B07327489	1
Caelo	Hidroclorotiazida	16F17-B07-327489	1
Caelo	Hidroclorotiazida	17H28-B01-340561	1
Caelo	Hidroclorotiazida	17L20-B02-345079	1
Caelo	Hidroclorotiazida	18017301	2
Caelo	Hidroclorotiazida	18017302	5
Caelo	Hidroclorotiazida	18017303	1
Caelo	Hidroclorotiazida	18017304	6
Caelo	Hidroclorotiazida	18017305	10
Caelo	Hidroclorotiazida	18017307	3
Caelo	Hidroclorotiazida	18108HCRII	1
Caelo	Hidroclorotiazida	182649005	1
Caelo	Hidroclorotiazida	18264901	7
Caelo	Hidroclorotiazida	18264904	7
Caelo	Hidroclorotiazida	18264907	6
Caelo	Hidroclorotiazida	1923280002	1
Caelo	Hidroclorotiazida	192328002	14
Caelo	Hidroclorotiazida	20004000002	9
Caelo	Hidroclorotiazida	20004000004	4
Caelo	Hidroclorotiazida	20004000007	2
Caelo	Hidroclorotiazida	20004000010	3
Caelo	Hidroclorotiazida	20004000011	2
Caelo	Hidroclorotiazida	2000400002	1
Caelo	Hidroclorotiazida	2000400004	1
Caelo	Hidroclorotiazida	2004000002	1
Caelo	Hidroclorotiazida	20E27-F01-371506	1
Caelo	Hidroclorotiazida	F01-3715006	1
Caeol/ Noweda	Hidroclorotiazida	15231009	2
Caesar & Loretz GmbH...	Hidroclorotiazida	18264907	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Hidroclorotiazida	192328002	1
Caesar & Loretz GmbH...	Hidroclorotiazida	20004000007	1
Caesar & Loretz GmbH...	Hidroclorotiazida	20004000004	1
Caesar & Loretz GmbH/Gehe	Hidroclorotiazida	18017304	1
Caesar & Loretz GmbH/Gehe	Hidroclorotiazida	18264904	1
Caesar & Loretz GmbH/Gehe	Hidroclorotiazida	18264906	1
Caesar & Loretz GmbH/Gehe	Hidroclorotiazida	18264907	1
Caesar & Loretz GmbH...	Hidroclorotiazida	18017307	1
Caesar & Loretz GmbH	Hidroclorotiazida	18017305	3
Caesar & Loretz GmbH	Hidroclorotiazida	18017307	1
Caesar & Loretz GmbH	Hidroclorotiazida	18264901	1
Caesar & Loretz GmbH	Hidroclorotiazida	18264904	4
Caesar & Loretz GmbH	Hidroclorotiazida	18264907	1
Caesar & Loretz GmbH	Hidroclorotiazida	192328002	14
Caesar & Loretz GmbH	Hidroclorotiazida	20004000002	5
Caesar & Loretz GmbH	Hidroclorotiazida	20004000003	1
Caesar & Loretz GmbH	Hidroclorotiazida	20004000004	1
Caesar & Loretz GmbH	Hidroclorotiazida	20004000007	4
Caesar & Loretz GmbH	Hidroclorotiazida	20004000010	1
Caesar & Loretz GmbH	Hidroclorotiazida	20004000011	1
Caesar & Loretz	Hidroclorotiazida	18017302	1
Fagron	Hidroclorotiazida		1
Fagron	Hidroclorotiazida	11E04-N10	1
Fagron	Hidroclorotiazida	11G12-N12	1
Fagron	Hidroclorotiazida	11l01-n02	2
Fagron	Hidroclorotiazida	11L01-N02	2
Fagron	Hidroclorotiazida	11L01-No2	1
Fagron	Hidroclorotiazida	11Lo1-No2	1
Fagron	Hidroclorotiazida	12A03-B40	3
Fagron	Hidroclorotiazida	12A03-B40-286110	1
Fagron	Hidroclorotiazida	12A03-B40-286111	3
Fagron	Hidroclorotiazida	12E04-N02	1
Fagron	Hidroclorotiazida	12L14-N11	4
Fagron	Hidroclorotiazida	13008504	1
Fagron	Hidroclorotiazida	13C25-N08	6
Fagron	Hidroclorotiazida	14B10B01	1
Fagron	Hidroclorotiazida	14B10-B01	2
Fagron	Hidroclorotiazida	14b10-b01-294558	1
Fagron	Hidroclorotiazida	14B10-B01-294558	6
Fagron	Hidroclorotiazida	14B10-B01-300822	2
Fagron	Hidroclorotiazida	14B10-B01-305043	3
Fagron	Hidroclorotiazida	15E04-B03	1
Fagron	Hidroclorotiazida	15E04-B03-309670	5
Fagron	Hidroclorotiazida	15K16	1
Fagron	Hidroclorotiazida	15K16-B01	4
Fagron	Hidroclorotiazida	15K16-B01-315836	3
Fagron	Hidroclorotiazida	15K16-B01-319833	9
Fagron	Hidroclorotiazida	16F17-B07	2
Fagron	Hidroclorotiazida	16F17-B07-322773	1
Fagron	Hidroclorotiazida	16F17-B07-324062	5
Fagron	Hidroclorotiazida	16F17-B07-327489	5
Fagron	Hidroclorotiazida	17038HCRII	1
Fagron	Hidroclorotiazida	17H28-B01340561	1
Fagron	Hidroclorotiazida	17H28-B01-340561	4
Fagron	Hidroclorotiazida	17L20-B02	1
Fagron	Hidroclorotiazida	17L20-B02-345079	5
Fagron	Hidroclorotiazida	17L20-B02-347789	6
Fagron	Hidroclorotiazida	17L20-B02-349593	6
Fagron	Hidroclorotiazida	17L20-B02-353429	4
Fagron	Hidroclorotiazida	17L20B02355636	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hidroclorotiazida	17L20-B02-355636	6
Fagron	Hidroclorotiazida	17L20B05	1
Fagron	Hidroclorotiazida	19100HCRII	1
Fagron	Hidroclorotiazida	19A04-B01	4
Fagron	Hidroclorotiazida	19A04-B01-359105	5
Fagron	Hidroclorotiazida	19a04-b01-363321	1
Fagron	Hidroclorotiazida	19A04-B01-363321	7
Fagron	Hidroclorotiazida	2002311234	1
Fagron	Hidroclorotiazida	20E27-F01	4
Fagron	Hidroclorotiazida	20E27-F01-371506	10
Fagron	Hidroclorotiazida	20E27-F01-373727	4
Fagron	Hidroclorotiazida	21H27-B04-216272	5
Fagron	Hidroclorotiazida	21H27-B04-220130	3
Fagron	Hidroclorotiazida	22K29-B01-224324	3
Fagron	Hidroclorotiazida	27101804	1
Fagron	Hidroclorotiazida	5013Q-03660	1
Fagron	Hidroclorotiazida	B04-2162702	1
Fagron	Hidroclorotiazida	C01-20150412	1
Fagron	Hidroclorotiazida	c01-20160510	1
Fagron	Hidroclorotiazida	C01-20160510	1
Fagron	Hidroclorotiazida	Co1-20150412	1
Fagron	Hidroclorotiazida	CQ1108	1
Fagron	Hidroclorotiazida	CR0601	1
Fagron	Hidroclorotiazida	F01-3737207	1
Fargon - Alliance He...	Hidroclorotiazida	17L20-B02-353429	1
Fargon/Phönix	Hidroclorotiazida	16F17-B07-327489	1
Fiebig	Hidroclorotiazida	115231003	1
Fiebig	Hidroclorotiazida	19100hcrII	1
Fiebig	Hidroclorotiazida	B01-3633201	1
Gehe	Hidroclorotiazida	12E04-N02	1
Gehe	Hidroclorotiazida	17L20-B02-353429	1
Gehe	Hidroclorotiazida	17L20-B02-355636	1
GEHE	Hidroclorotiazida	18017302	1
Gehe	Hidroclorotiazida	18017304	1
Gehe	Hidroclorotiazida	23002418002	1
Kehr	Hidroclorotiazida	20004000011	1
Kehr	Hidroclorotiazida	23A04-B06-229298	1
noweda	Hidroclorotiazida	15231009	1
Noweda	Hidroclorotiazida	16269307	1
Noweda	Hidroclorotiazida	23A04-B06-229298	2
Phoenix	Hidroclorotiazida	15231003	1
Phoenix	Hidroclorotiazida	17L20-B02-347789	1
Phoenix	Hidroclorotiazida	18017302	2
Phoenix	Hidroclorotiazida	18264901	1
Phoenix	Hidroclorotiazida	18264904	2
Phönix	Hidroclorotiazida	192328002	1
Sanacorp	Hidroclorotiazida	12A03-B40-26111	1
Sanacorp	Hidroclorotiazida	15231008	1
Sanacorp	Hidroclorotiazida	16269302	1
Sanacorp	Hidroclorotiazida	18017302	1
Sanacorp	Hidroclorotiazida	19A04-B01	2
Sanacorp	Hidroclorotiazida	22K29-B01-224324	1
Sanacorp	Hidroclorotiazida	23A04-B06-233623	1

- 235 627 spectra from 1515 *Apo-Ident* customers from a total of 49 138 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Hidroclorotiazida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidroclorotiazida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	200	0	201 884
Type C	0	430	10	235 627

The substance/substance group *Hidroclorotiazida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	97.7273 % (> 97.0455 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20888	21589	16,49	313,30
21589	21589	0,00	318,78
23989	24362	5,89	323,75
24362	24362	0,00	324,85
25590	24362	5,39	322,87
26172	24362	9,40	322,94

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidrocortisona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20006-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidrocortisona; Hydrocortisonum

Special notes

When selecting the *Hidrocortisona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidrocortisona	9	11	544

Second-stage model

For differentiation of the substance/substance group *Hidrocortisona* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidrocortisona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	83,00	–
⋮	⋮	⋮
Furoato de mometasona	>50	117,19
Escina, hidrossolúvel	>50	157,42
Sorbato de potássio	>50	170,67
Citrato monobásico de magnésio, hid…	>50	180,36
Sulfato de atropina	>50	221,65
Quinolina amarela	>50	373,09
Orotato de cálcio di-hidratado	>50	487,26
Cloridrato de propranolol	>50	571,76
Sacarina sódica	>50	609,19
Fenitoína	>50	850,49

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidrocortisona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidrocortisona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidrocortisona	13341502	21461	60	20131203
Caelo	Hidrocortisona	13341502	21463	60	20131203
Caelo	Hidrocortisona	180915	24020	40	20180412*
Euro OTC	Hidrocortisona	1206018-01	21293	40	20130727
Euro OTC	Hidrocortisona	1509029	21899	60	20151014*
Euro OTC	Hidrocortisona	1509029	21899SI	51	20151014*
Euro OTC	Hidrocortisona	1611016	22910	40	20161220*
Euro OTC	Hidrocortisona	2101003	25571	40	20210128*
Euro OTC	Hidrocortisona	2101003	25571SI	40	20210128*
Fagron	Hidrocortisona	16A19-B06-320970	22829	40	20160204

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hidrocortisona	16A19-B06-320970	22829SI	30	20160204
Fagron	Hidrocortisona	16A19-B06-321981	22837	40	20160204
Fagron	Hidrocortisona	16A19-B06-321981	22838	40	1702302
Fagron	Hidrocortisona	16H01-B01-326071	22928	40	20160907
Fagron	Hidrocortisona	16H01-B01-326071	22928SI	40	20160907

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 661 spectra of 15 reference samples from the substance/substance group *Hidrocortisona*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 301 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1119 spectra of 29 reference samples from the substance/substance group *Hidrocortisona*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidrocortisona	160952	22778	40
Caelo	Hidrocortisona	171194	23340	20
Caelo	Hidrocortisona	172566	23840	40
Caelo	Hidrocortisona	183243	24521	40
Caelo	Hidrocortisona	21001215005	25926	40
Caelo	Hidrocortisona	22003779	27250	40
Euro OTC	Hidrocortisona	1802009	23945	40
Euro OTC	Hidrocortisona	1906033	24771	40
Euro OTC	Hidrocortisona	2205003	26213	40
Euro OTC	Hidrocortisona	2401017	27152	40
Fagron	Hidrocortisona	22E09-B02-220942	26395	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidrocortisona	13341502	21463SI†	60
Caelo	Hidrocortisona	160952	22778SI	40
Caelo	Hidrocortisona	171194	23340SI	28
Caelo	Hidrocortisona	171194	23659	40
Caelo	Hidrocortisona	171194	23659SI	30
Caelo	Hidrocortisona	172566	23840SI	40
Caelo	Hidrocortisona	180915	24020SI†	40
Caelo	Hidrocortisona	183243	24521SI	40
Caelo	Hidrocortisona	21001215005	25926SI	40
Caelo	Hidrocortisona	22003779	27250SI	40
Euro OTC	Hidrocortisona	1611016	22910SI†	40
Euro OTC	Hidrocortisona	1802009	23945SI	40
Euro OTC	Hidrocortisona	1906033	24771SI	40
Euro OTC	Hidrocortisona	2205003	26213SI	40
Euro OTC	Hidrocortisona	2401017	27152SI	40
Fagron	Hidrocortisona	16A19-B06-321981	22837SI†	30
Fagron	Hidrocortisona	16A19-B06-321981	22838SI†	31
Fagron	Hidrocortisona	22E09-B02-220942	26395SI	40

- 200 965 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4496 spectra from 1108 *Apo-Ident* customers from 564 batches from the substance/substance group *Hidrocortisona*.
- Among them are spectra of independent samples from 544 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hidrocortisona	2100121029	1
	Hidrocortisona	21001215017	2
	Hidrocortisona	21001215018	2
	Hidrocortisona	21001215019	2
	Hidrocortisona	21001215023	3
	Hidrocortisona	21001215026	2
	Hidrocortisona	21001215027	3
	Hidrocortisona	21001215029	7
	Hidrocortisona	21001215030	7
	Hidrocortisona	21001215032	3
	Hidrocortisona	21001215034	10
	Hidrocortisona	21001215035	3
	Hidrocortisona	21001215036	4
	Hidrocortisona	2200377900	1
	Hidrocortisona	22003779003	2
	Hidrocortisona	22003779004	17

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Hidrocortisona	22003779005	4
	Hidrocortisona	22003779006	18
	Hidrocortisona	22003779008	2
	Hidrocortisona	22003779011	1
	Hidrocortisona	22003779012	3
	Hidrocortisona	220500301	1
	Hidrocortisona	2205003-01	8
	Hidrocortisona	22E09-B02-219558	1
	Hidrocortisona	23003407002	1
	Hidrocortisona	23D06-B01-232991	1
	Hidrocortisona	K05M20211103	1
/ AHD	Hidrocortisona	16095202	1
A.H. 10.06.13 ek: 10,01EUR	Hidrocortisona	1204037-01	1
AEP	Hidrocortisona	21001215015	1
AEP	Hidrocortisona	21001215032	1
AHC 02.09.13 EK9,85	Hidrocortisona	1112030-01	1
AHC	Hidrocortisona	22003779006	1
ahd,11,95EUR 10.04.14	Hidrocortisona	13341504-07R07	1
AHD/Euro	Hidrocortisona	1802009	1
AHD/Euro	Hidrocortisona	1802009-01	2
AHD	Hidrocortisona	13069507	1
AHD	Hidrocortisona	18091503	1
AHD	Hidrocortisona	18091520	1
AHD	Hidrocortisona	21001215021	2
AHD	Hidrocortisona	21001215032	1
AHD	Hidrocortisona	22003779004	1
AHD	Hidrocortisona	22003779011	2
AHD	Hidrocortisona	2205003-01	1
AHD;19.06.15;18,70EUR	Hidrocortisona	14301306	1
AHL	Hidrocortisona	15125-B01-313084	1
Alliance Healtcare	Hidrocortisona	192241008	1
Alliance Healtcare	Hidrocortisona	21001215018	1
Alliance Health 11.0...	Hidrocortisona	1315505	1
Alliance Health25.04.2014	Hidrocortisona	13341503	3
Alliance Healthcare	Hidrocortisona	192241005	1
Alliance	Hidrocortisona	21001215021	1
Allianz Healthcare	Hidrocortisona	1509029-01	1
Allianz Healthcare	Hidrocortisona	1802009-01	1
Anzag 14.12.12 ek:10,01	Hidrocortisona	1202032-01	1
Anzag ek:10.01EUR 18.07.12	Hidrocortisona	1107005-03	1
Anzag	Hidrocortisona	1107005-02	1
Anzag	Hidrocortisona	11260305	1
Anzag	Hidrocortisona	1206018-01	1
Anzag	Hidrocortisona	12104307	1
Anzag	Hidrocortisona	14301306	1
Anzag	Hidrocortisona	1501034-01	1
Anzag	Hidrocortisona	1505016-01	1
Anzag	Hidrocortisona	1509229-01	1
Anzag	Hidrocortisona	183243006	1
Anzag	Hidrocortisona	192241007	1
Anzag	Hidrocortisona	19224107	1
Anzag	Hidrocortisona	20004116003	2
Anzag	Hidrocortisona	20004116007	1
Anzag	Hidrocortisona	21001215019	1
Beiersdorf/ Vedono	Hidrocortisona	15181004	1
Berkel AHK	Hidrocortisona	14301305	1
Bionorica	Hidrocortisona	16004604	1
Bombastus	Hidrocortisona	14I05-B02-300227	1
cae	Hidrocortisona	18324307	1
Caeelo	Hidrocortisona	17090005	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
cael	Hidrocortisona	183243002	1
Caelo	Hidrocortisona		2
Caelo	Hidrocortisona	10071704	1
Caelo	Hidrocortisona	10282208	1
Caelo	Hidrocortisona	11021302	1
Caelo	Hidrocortisona	1109845	1
Caelo	Hidrocortisona	11260308	3
Caelo	Hidrocortisona	11260309	3
Caelo	Hidrocortisona	11273704	1
Caelo	Hidrocortisona	113I-01719	1
Caelo	Hidrocortisona	1140317	1
Caelo	Hidrocortisona	1190218/17256602	1
Caelo	Hidrocortisona	120403701	1
Caelo	Hidrocortisona	12104301	1
Caelo	Hidrocortisona	12104303	5
Caelo	Hidrocortisona	12104304	6
Caelo	Hidrocortisona	12104305	3
Caelo	Hidrocortisona	12104306	9
Caelo	Hidrocortisona	12104307	17
Caelo	Hidrocortisona	12104308	8
Caelo	Hidrocortisona	12104309	2
Caelo	Hidrocortisona	12119303	8
Caelo	Hidrocortisona	12119304	4
Caelo	Hidrocortisona	12167001	7
Caelo	Hidrocortisona	12167007	10
Caelo	Hidrocortisona	12167010	10
Caelo	Hidrocortisona	12167010-3437311151	1
Caelo	Hidrocortisona	1216707	1
Caelo	Hidrocortisona	12k08-n01	1
Caelo	Hidrocortisona	130617H	1
Caelo	Hidrocortisona	13063501	1
Caelo	Hidrocortisona	1306906	1
Caelo	Hidrocortisona	13069501	10
Caelo	Hidrocortisona	13069502	5
Caelo	Hidrocortisona	13069505	4
Caelo	Hidrocortisona	13069506	8
Caelo	Hidrocortisona	13069507	4
Caelo	Hidrocortisona	13069509	2
Caelo	Hidrocortisona	13069510	6
Caelo	Hidrocortisona	13155601	9
Caelo	Hidrocortisona	13155602	8
Caelo	Hidrocortisona	13155603	12
Caelo	Hidrocortisona	13155604	8
Caelo	Hidrocortisona	13155605	3
Caelo	Hidrocortisona	13155611	2
Caelo	Hidrocortisona	13155614	3
Caelo	Hidrocortisona	133341502	1
Caelo	Hidrocortisona	13341501	7
Caelo	Hidrocortisona	13341502	11
Caelo	Hidrocortisona	13341503	1
Caelo	Hidrocortisona	13341504	7
Caelo	Hidrocortisona	13341508	4
Caelo	Hidrocortisona	13341509	8
Caelo	Hidrocortisona	13341510	12
Caelo	Hidrocortisona	13341511	5
Caelo	Hidrocortisona	13342504	1
Caelo	Hidrocortisona	140301305	1
Caelo	Hidrocortisona	14115103	2
Caelo	Hidrocortisona	14115104	1
Caelo	Hidrocortisona	14115105	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrocortisona	14115107	11
Caelo	Hidrocortisona	14115108	2
Caelo	Hidrocortisona	14301304	4
Caelo	Hidrocortisona	14301305	5
Caelo	Hidrocortisona	14301306	6
Caelo	Hidrocortisona	14301307	2
Caelo	Hidrocortisona	14301310	14
Caelo	Hidrocortisona	14301311	10
Caelo	Hidrocortisona	14301312	8
Caelo	Hidrocortisona	14301313	6
Caelo	Hidrocortisona	14b04-B02-293422	1
Caelo	Hidrocortisona	15/25-B01-318486	1
Caelo	Hidrocortisona	1501034-01	2
Caelo	Hidrocortisona	15021104	7
Caelo	Hidrocortisona	15021105	7
Caelo	Hidrocortisona	15021106	3
Caelo	Hidrocortisona	15021107	11
Caelo	Hidrocortisona	1505016-01	3
Caelo	Hidrocortisona	1509029-01	5
Caelo	Hidrocortisona	1518012	1
Caelo	Hidrocortisona	1518013	1
Caelo	Hidrocortisona	15181003	11
Caelo	Hidrocortisona	15181004	11
Caelo	Hidrocortisona	15181006	20
Caelo	Hidrocortisona	15181007	5
Caelo	Hidrocortisona	15181008	2
Caelo	Hidrocortisona	15181012	16
Caelo	Hidrocortisona	15181012/20160309/10	1
Caelo	Hidrocortisona	15181013	11
Caelo	Hidrocortisona	15181014	6
Caelo	Hidrocortisona	15216101	10
Caelo	Hidrocortisona	15278702	11
Caelo	Hidrocortisona	15278703	9
Caelo	Hidrocortisona	15278705	11
Caelo	Hidrocortisona	15278706	6
Caelo	Hidrocortisona	16004603	14
Caelo	Hidrocortisona	16004604	28
Caelo	Hidrocortisona	16004605	14
Caelo	Hidrocortisona	16004607	16
Caelo	Hidrocortisona	16004608	12
Caelo	Hidrocortisona	16004611	11
Caelo	Hidrocortisona	16004612	16
Caelo	Hidrocortisona	16004612/2020317	1
Caelo	Hidrocortisona	16041801	1
Caelo	Hidrocortisona	16095201	27
Caelo	Hidrocortisona	16095202	12
Caelo	Hidrocortisona	16095203	10
Caelo	Hidrocortisona	16095207	8
Caelo	Hidrocortisona	16095209	7
Caelo	Hidrocortisona	16095210	24
Caelo	Hidrocortisona	16095212	8
Caelo	Hidrocortisona	16095213	13
Caelo	Hidrocortisona	16095213-20170704Ma7	1
Caelo	Hidrocortisona	16098201	2
Caelo	Hidrocortisona	1611016	1
Caelo	Hidrocortisona	1611016-01	5
Caelo	Hidrocortisona	16255603	10
Caelo	Hidrocortisona	16255604	2
Caelo	Hidrocortisona	16255606	1
Caelo	Hidrocortisona	16255607	13

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrocortisona	16255608	15
Caelo	Hidrocortisona	16255608NP	1
Caelo	Hidrocortisona	16255680	1
Caelo	Hidrocortisona	1626-B04-330340	1
Caelo	Hidrocortisona	16272304	13
Caelo	Hidrocortisona	16272305	11
Caelo	Hidrocortisona	16272306	14
Caelo	Hidrocortisona	16272308	5
Caelo	Hidrocortisona	1627231	1
Caelo	Hidrocortisona	16272311	7
Caelo	Hidrocortisona	1672305	1
Caelo	Hidrocortisona	1672308	1
Caelo	Hidrocortisona	167272306	1
Caelo	Hidrocortisona	17090003	4
Caelo	Hidrocortisona	17090004	1
Caelo	Hidrocortisona	17090005	8
Caelo	Hidrocortisona	170921HA/17090003	1
Caelo	Hidrocortisona	1711940	1
Caelo	Hidrocortisona	17119402	21
Caelo	Hidrocortisona	17119403	24
Caelo	Hidrocortisona	17119404	1
Caelo	Hidrocortisona	17119405	36
Caelo	Hidrocortisona	17119406	23
Caelo	Hidrocortisona	17119407	31
Caelo	Hidrocortisona	17119410	7
Caelo	Hidrocortisona	1719402-20171106Ma2	1
Caelo	Hidrocortisona	1719405	1
Caelo	Hidrocortisona	17229410	1
Caelo	Hidrocortisona	17256602	56
Caelo	Hidrocortisona	17256603	10
Caelo	Hidrocortisona	17256604	36
Caelo	Hidrocortisona	17256605	26
Caelo	Hidrocortisona	17256607	15
Caelo	Hidrocortisona	17256804	1
Caelo	Hidrocortisona	1726602	1
Caelo	Hidrocortisona	1726603	1
Caelo	Hidrocortisona	1731205	1
Caelo	Hidrocortisona	173512	1
Caelo	Hidrocortisona	173512005	1
Caelo	Hidrocortisona	17351202	19
Caelo	Hidrocortisona	17351203	36
Caelo	Hidrocortisona	17351205	65
Caelo	Hidrocortisona	17351206	11
Caelo	Hidrocortisona	17351209	11
Caelo	Hidrocortisona	17351209-20180830Ma3	1
Caelo	Hidrocortisona	17351210	2
Caelo	Hidrocortisona	1735123	1
Caelo	Hidrocortisona	17526602	1
Caelo	Hidrocortisona	1756602	1
Caelo	Hidrocortisona	17E10-B04-334857	1
Caelo	Hidrocortisona	18002009-01	1
Caelo	Hidrocortisona	1802009-01	3
Caelo	Hidrocortisona	1802009-1	2
Caelo	Hidrocortisona	18031508	1
Caelo	Hidrocortisona	18042601	1
Caelo	Hidrocortisona	18061802	1
Caelo	Hidrocortisona	18062003	1
Caelo	Hidrocortisona	18091501	27
Caelo	Hidrocortisona	18091501-H20181115Ma	3
Caelo	Hidrocortisona	18091502	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrocortisona	18091503	36
Caelo	Hidrocortisona	18091505	38
Caelo	Hidrocortisona	18091506	30
Caelo	Hidrocortisona	18091507	33
Caelo	Hidrocortisona	18091508	8
Caelo	Hidrocortisona	18091519	41
Caelo	Hidrocortisona	18091520	36
Caelo	Hidrocortisona	180915208	1
Caelo	Hidrocortisona	18091521	2
Caelo	Hidrocortisona	18091524	22
Caelo	Hidrocortisona	18091525	44
Caelo	Hidrocortisona	180915252	1
Caelo	Hidrocortisona	18091526	6
Caelo	Hidrocortisona	18091528	22
Caelo	Hidrocortisona	18091530	1
Caelo	Hidrocortisona	18091531	18
Caelo	Hidrocortisona	18091531x2	1
Caelo	Hidrocortisona	180915321	1
Caelo	Hidrocortisona	180921531	1
Caelo	Hidrocortisona	18121713	1
Caelo	Hidrocortisona	1824311	1
Caelo	Hidrocortisona	1832243006	1
Caelo	Hidrocortisona	18323006	1
Caelo	Hidrocortisona	18324207	1
Caelo	Hidrocortisona	183243002	58
Caelo	Hidrocortisona	183243003	7
Caelo	Hidrocortisona	183243004	19
Caelo	Hidrocortisona	183243006	54
Caelo	Hidrocortisona	18324301	32
Caelo	Hidrocortisona	18324302	28
Caelo	Hidrocortisona	18324303	6
Caelo	Hidrocortisona	18324306	34
Caelo	Hidrocortisona	18324307	31
Caelo	Hidrocortisona	18324308	24
Caelo	Hidrocortisona	18324310	9
Caelo	Hidrocortisona	18324311	27
Caelo	Hidrocortisona	186324307	1
Caelo	Hidrocortisona	1891528	1
Caelo	Hidrocortisona	1907151621	1
Caelo	Hidrocortisona	19224002	1
Caelo	Hidrocortisona	19224100	1
Caelo	Hidrocortisona	192241002	5
Caelo	Hidrocortisona	192241004	15
Caelo	Hidrocortisona	192241005	30
Caelo	Hidrocortisona	192241007	24
Caelo	Hidrocortisona	192241008	70
Caelo	Hidrocortisona	200004116007	2
Caelo	Hidrocortisona	20004106005	1
Caelo	Hidrocortisona	200041116003	1
Caelo	Hidrocortisona	20004116001	35
Caelo	Hidrocortisona	20004116002	11
Caelo	Hidrocortisona	20004116003	29
Caelo	Hidrocortisona	20004116004	32
Caelo	Hidrocortisona	20004116005	22
Caelo	Hidrocortisona	20004116006	24
Caelo	Hidrocortisona	20004116007	16
Caelo	Hidrocortisona	20004278004	1
Caelo	Hidrocortisona	2004116006	1
Caelo	Hidrocortisona	200411606	1
Caelo	Hidrocortisona	2013U-01719	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrocortisona	2100115007	1
Caelo	Hidrocortisona	21001215003	3
Caelo	Hidrocortisona	21001215004	15
Caelo	Hidrocortisona	21001215005	37
Caelo	Hidrocortisona	21001215006	23
Caelo	Hidrocortisona	21001215007	24
Caelo	Hidrocortisona	21001215009	1
Caelo	Hidrocortisona	21001215010	28
Caelo	Hidrocortisona	21001215011	12
Caelo	Hidrocortisona	21001215013	29
Caelo	Hidrocortisona	21001215014	20
Caelo	Hidrocortisona	21001215015	7
Caelo	Hidrocortisona	21001215017	10
Caelo	Hidrocortisona	21001215018	13
Caelo	Hidrocortisona	21001215019	13
Caelo	Hidrocortisona	21001215020	12
Caelo	Hidrocortisona	21001215021	23
Caelo	Hidrocortisona	21001215023	3
Caelo	Hidrocortisona	21001215026	2
Caelo	Hidrocortisona	21001215027	2
Caelo	Hidrocortisona	21001215029	1
Caelo	Hidrocortisona	2100125014	1
Caelo	Hidrocortisona	210012515010	1
Caelo	Hidrocortisona	2100215013	1
Caelo	Hidrocortisona	210922(20004116002)	1
Caelo	Hidrocortisona	21101303	1
Caelo	Hidrocortisona	211029(21001215003)	1
Caelo	Hidrocortisona	211115(21001215003)	1
Caelo	Hidrocortisona	211123(21001215003)	2
Caelo	Hidrocortisona	211130(21001215003)	1
Caelo	Hidrocortisona	211227(21001215003)	1
Caelo	Hidrocortisona	2180917/16255608	1
Caelo	Hidrocortisona	220037789006	1
Caelo	Hidrocortisona	22003779005	2
Caelo	Hidrocortisona	22003779008	1
Caelo	Hidrocortisona	220118(21001215003)	1
Caelo	Hidrocortisona	220120	1
Caelo	Hidrocortisona	220127	1
Caelo	Hidrocortisona	220210(21001215003)	1
Caelo	Hidrocortisona	220413(21001215003)	1
Caelo	Hidrocortisona	2205003-01	4
Caelo	Hidrocortisona	220510(21001215009)	1
Caelo	Hidrocortisona	220519(21001215003)	1
Caelo	Hidrocortisona	220905(21001215015)	1
Caelo	Hidrocortisona	260416v4	1
Caelo	Hidrocortisona	27101801	1
Caelo	Hidrocortisona	2760	1
Caelo	Hidrocortisona	3081604	1
Caelo	Hidrocortisona	31032014D	1
Caelo	Hidrocortisona	3110396	1
Caelo	Hidrocortisona	3110456	1
Caelo	Hidrocortisona	39/AKD17	1
Caelo	Hidrocortisona	3912Q-01719	1
Caelo	Hidrocortisona	4817Q-01719	1
Caelo	Hidrocortisona	7082004	1
Caelo	Hidrocortisona	7101301	1
Caelo	Hidrocortisona	8041701	1
Caelo	Hidrocortisona	810911	1
Caelo	Hidrocortisona	8717	1
Caelo	Hidrocortisona	9271205	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidrocortisona	B02-2005104	1
Caelo	Hidrocortisona	caelo	1
Caelo	Hidrocortisona	Caelo21001215003	2
Caelo	Hidrocortisona	K05B20160909	1
Caeol/Noweda	Hidrocortisona	16095212	1
Caeolo/Krieger	Hidrocortisona	17119406	1
Caesar & Lorenz GmbH	Hidrocortisona	15181004	1
Caesar & Lorenz	Hidrocortisona	21001215026	1
Caesar & Loretz /Phönix	Hidrocortisona	21001215003	1
Caesar & Loretz /Sanacorp	Hidrocortisona	21001215011	2
Caesar & Loretz GmbH...	Hidrocortisona	21001215006	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215014	1
Caesar & Loretz GmbH...	Hidrocortisona	183243006	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116001	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215021	1
Caesar & Loretz GmbH...	Hidrocortisona	18324306	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116001	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116004	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH...	Hidrocortisona	183243006	1
Caesar & Loretz GmbH...	Hidrocortisona	18324307	1
Caesar & Loretz GmbH...	Hidrocortisona	18324308	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116003	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH...	Hidrocortisona	18324211	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215005	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215023	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116002	1
Caesar & Loretz GmbH...	Hidrocortisona	183243002	1
Caesar & Loretz GmbH...	Hidrocortisona	18324311	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215009	1
Caesar & Loretz GmbH/AEP	Hidrocortisona	18091525	1
Caesar & Loretz GmbH/AEP	Hidrocortisona	21001215011	1
Caesar & Loretz GmbH/AHD	Hidrocortisona	20004116004	1
Caesar & Loretz GmbH/AHD	Hidrocortisona	21001215011	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116001	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215007	1
Caesar & Loretz GmbH...	Hidrocortisona	183243006	1
Caesar & Loretz GmbH...	Hidrocortisona	18091508	1
Caesar & Loretz GmbH...	Hidrocortisona	183243003	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH/G	Hidrocortisona	192241007	1
Caesar & Loretz GmbH/G	Hidrocortisona	21001215004	1
Caesar & Loretz GmbH/G	Hidrocortisona	21001215011	1
Caesar & Loretz GmbH/GEHE	Hidrocortisona	192241008	1
Caesar & Loretz GmbH/Gehe	Hidrocortisona	20004116005	1
Caesar & Loretz GmbH/Gehe	Hidrocortisona	21001215004	2
Caesar & Loretz GmbH/Gehe	Hidrocortisona	21001215023	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215005	2
Caesar & Loretz GmbH...	Hidrocortisona	18324302	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116006	2
Caesar & Loretz GmbH...	Hidrocortisona	21001215006	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215020	2
Caesar & Loretz GmbH...	Hidrocortisona	18091524	1
Caesar & Loretz GmbH...	Hidrocortisona	183243004	1
Caesar & Loretz GmbH...	Hidrocortisona	18324306	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116005	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Hidrocortisona	21001215004	2
Caesar & Loretz GmbH...	Hidrocortisona	21001215007	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215010	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215013	1
Caesar & Loretz GmbH/Kehr	Hidrocortisona	183243006	1
Caesar & Loretz GmbH/Kehr	Hidrocortisona	18324301	1
Caesar & Loretz GmbH/Kehr	Hidrocortisona	18324306	1
Caesar & Loretz GmbH/Kehr	Hidrocortisona	18324308	1
Caesar & Loretz GmbH/Kehr	Hidrocortisona	20004116007	1
Caesar & Loretz GmbH...	Hidrocortisona	183243002	2
Caesar & Loretz GmbH...	Hidrocortisona	20004116001	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215005	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215006	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215010	1
Caesar & Loretz GmbH...	Hidrocortisona	183243003	2
Caesar & Loretz GmbH...	Hidrocortisona	18324302	1
Caesar & Loretz GmbH...	Hidrocortisona	192241005	2
Caesar & Loretz GmbH...	Hidrocortisona	20004116006	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116007	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215020	1
Caesar & Loretz GmbH/Otto	Hidrocortisona	18324307	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116002	2
Caesar & Loretz GmbH/Phoe	Hidrocortisona	20004116004	1
Caesar & Loretz GmbH...	Hidrocortisona	18324302	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116003	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215010	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215021	1
Caesar & Loretz GmbH...	Hidrocortisona	18091520	1
Caesar & Loretz GmbH...	Hidrocortisona	183243003	2
Caesar & Loretz GmbH...	Hidrocortisona	183243006	1
Caesar & Loretz GmbH...	Hidrocortisona	18324301	1
Caesar & Loretz GmbH...	Hidrocortisona	192241005	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116002	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116003	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116005	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215003	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215006	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215007	2
Caesar & Loretz GmbH...	Hidrocortisona	21001215013	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215014	1
Caesar & Loretz GmbH/Sa	Hidrocortisona	18324302	1
Caesar & Loretz GmbH/Sana	Hidrocortisona	20004116004	1
Caesar & Loretz GmbH/Sana	Hidrocortisona	21001215006	1
Caesar & Loretz GmbH...	Hidrocortisona	183243002	1
Caesar & Loretz GmbH...	Hidrocortisona	192241004	1
Caesar & Loretz GmbH...	Hidrocortisona	192241008	1
Caesar & Loretz GmbH...	Hidrocortisona	20004116003	3
Caesar & Loretz GmbH...	Hidrocortisona	21001215007	2
Caesar & Loretz GmbH...	Hidrocortisona	21001215013	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215014	1
Caesar & Loretz GmbH...	Hidrocortisona	21001215017	1
Caesar & Loretz GmbH	Hidrocortisona	12167010	1
Caesar & Loretz GmbH	Hidrocortisona	13069506	1
Caesar & Loretz GmbH	Hidrocortisona	13069507	1
Caesar & Loretz GmbH	Hidrocortisona	15021107	1
Caesar & Loretz GmbH	Hidrocortisona	15181012	1
Caesar & Loretz GmbH	Hidrocortisona	16004612	1
Caesar & Loretz GmbH	Hidrocortisona	17256605	1
Caesar & Loretz GmbH	Hidrocortisona	17351205	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hidrocortisona	17351210	3
Caesar & Loretz GmbH	Hidrocortisona	18091505	1
Caesar & Loretz GmbH	Hidrocortisona	18091506	4
Caesar & Loretz GmbH	Hidrocortisona	18091507	1
Caesar & Loretz GmbH	Hidrocortisona	18091519	6
Caesar & Loretz GmbH	Hidrocortisona	18091520	10
Caesar & Loretz GmbH	Hidrocortisona	18091524	3
Caesar & Loretz GmbH	Hidrocortisona	18091525	6
Caesar & Loretz GmbH	Hidrocortisona	18091526	3
Caesar & Loretz GmbH	Hidrocortisona	18091528	6
Caesar & Loretz GmbH	Hidrocortisona	18091531	4
Caesar & Loretz GmbH	Hidrocortisona	183243002	11
Caesar & Loretz GmbH	Hidrocortisona	183243004	13
Caesar & Loretz GmbH	Hidrocortisona	183243006	12
Caesar & Loretz GmbH	Hidrocortisona	18324301	6
Caesar & Loretz GmbH	Hidrocortisona	18324302	12
Caesar & Loretz GmbH	Hidrocortisona	18324303	1
Caesar & Loretz GmbH	Hidrocortisona	18324306	13
Caesar & Loretz GmbH	Hidrocortisona	18324307	13
Caesar & Loretz GmbH	Hidrocortisona	18324308	8
Caesar & Loretz GmbH	Hidrocortisona	18324310	4
Caesar & Loretz GmbH	Hidrocortisona	18324311	9
Caesar & Loretz GmbH	Hidrocortisona	192241002	8
Caesar & Loretz GmbH	Hidrocortisona	192241003	1
Caesar & Loretz GmbH	Hidrocortisona	192241004	1
Caesar & Loretz GmbH	Hidrocortisona	192241005	3
Caesar & Loretz GmbH	Hidrocortisona	192241007	11
Caesar & Loretz GmbH	Hidrocortisona	192241008	20
Caesar & Loretz GmbH	Hidrocortisona	19K05-B02-195614	1
Caesar & Loretz GmbH	Hidrocortisona	20000978010	1
Caesar & Loretz GmbH	Hidrocortisona	20004116001	16
Caesar & Loretz GmbH	Hidrocortisona	20004116002	5
Caesar & Loretz GmbH	Hidrocortisona	20004116003	15
Caesar & Loretz GmbH	Hidrocortisona	20004116004	12
Caesar & Loretz GmbH	Hidrocortisona	20004116005	2
Caesar & Loretz GmbH	Hidrocortisona	20004116006	15
Caesar & Loretz GmbH	Hidrocortisona	20004116007	7
Caesar & Loretz GmbH	Hidrocortisona	20B17-B02-200514	1
Caesar & Loretz GmbH	Hidrocortisona	21001215003	2
Caesar & Loretz GmbH	Hidrocortisona	21001215004	10
Caesar & Loretz GmbH	Hidrocortisona	21001215005	10
Caesar & Loretz GmbH	Hidrocortisona	21001215006	6
Caesar & Loretz GmbH	Hidrocortisona	21001215007	7
Caesar & Loretz GmbH	Hidrocortisona	21001215009	2
Caesar & Loretz GmbH	Hidrocortisona	21001215010	10
Caesar & Loretz GmbH	Hidrocortisona	21001215011	9
Caesar & Loretz GmbH	Hidrocortisona	21001215013	7
Caesar & Loretz GmbH	Hidrocortisona	21001215014	9
Caesar & Loretz GmbH	Hidrocortisona	21001215015	2
Caesar & Loretz GmbH	Hidrocortisona	21001215016	1
Caesar & Loretz GmbH	Hidrocortisona	21001215017	1
Caesar & Loretz GmbH	Hidrocortisona	21001215018	2
Caesar & Loretz GmbH	Hidrocortisona	21001215019	9
Caesar & Loretz GmbH	Hidrocortisona	21001215020	5
Caesar & Loretz GmbH	Hidrocortisona	21001215021	5
Caesar & Loretz GmbH	Hidrocortisona	21001215023	5
Caesar & Loretz GmbH	Hidrocortisona	21001215028	1
Caesar & Loretz GmbH	Hidrocortisona	21001215029	1
Caesar & Loretz GmbH	Hidrocortisona	21001215030	2
Caesar & Loretz GmbH	Hidrocortisona	21001215035	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hidrocortisona	22003779004	1
Caesar & Loretz GmbH	Hidrocortisona	22003779006	1
Caesar & Loretz GmbH	Hidrocortisona	B02-1956104	1
Caesar & Loretz GmbH...	Hidrocortisona	192241007	1
Caesar & Loretz Hild...	Hidrocortisona	192241004	1
Caesar & Loretz Hilden	Hidrocortisona	18091520	1
Caesar & Loretz Hilden	Hidrocortisona	183243002	1
Caesar & Loretz Hilden	Hidrocortisona	183243006	1
Caesar & Loretz Hilden	Hidrocortisona	18324306	1
Caesar & Loretz/ Gei...	Hidrocortisona	18091520	1
Caesar & Loretz/Geil...	Hidrocortisona	18091528	1
Caesar & Loretz/Noweda	Hidrocortisona	192241005	1
Caesar & Loretz/Phoenix	Hidrocortisona	21001215006	1
Caesar & Loretz	Hidrocortisona	16095201	1
Caesar & Loretz	Hidrocortisona	16255603	1
Caesar & Loretz	Hidrocortisona	17256603	2
Caesar & Loretz	Hidrocortisona	192241008	1
Caesar / Phönix 22.0...	Hidrocortisona	20004116007	1
Caesar&Lorenz	Hidrocortisona	20004116003	1
Caesar&Loretz GmbH,A...	Hidrocortisona	16272305	1
Caesar&Loretz GmbH	Hidrocortisona	12104308	1
Caesar&Loretz GmbH	Hidrocortisona	21001215020	1
Caesar&loretz,Phoenix	Hidrocortisona	15021105	1
Caesar&loretz,Phoenix	Hidrocortisona	15181004	1
Caesar/Alliance Heal...	Hidrocortisona	20004116004	1
Caleo/ Noweda	Hidrocortisona	17351203	2
Cealo / Anzag	Hidrocortisona	220322(21001215003)	1
Cealo / Anzag	Hidrocortisona	220419(21001215003)	1
Cealo / Anzag	Hidrocortisona	220531(21001215003)	1
Cealo / Anzag	Hidrocortisona	220712(21001215003)	1
Cealo, Anzag 26.08.19	Hidrocortisona	18091528	1
Cealo/ Anzag	Hidrocortisona	16095210	1
Cealo/ Noweda	Hidrocortisona	17351209	1
Cealo/Jenne	Hidrocortisona	211019(21001215003)	2
Cealo/Jenne	Hidrocortisona	211104(20004116005)	2
Cealo/Sanacorp	Hidrocortisona	20004116004	1
Cealo	Hidrocortisona	16004612	1
Cealo	Hidrocortisona	17119405	1
Cealo	Hidrocortisona	18091503	1
Cealo	Hidrocortisona	18091505	1
Cealo	Hidrocortisona	192241004	1
Celo/AHD	Hidrocortisona	18091506	1
Delta	Hidrocortisona	16H01-B01-326071	1
Ebert & Jacobi	Hidrocortisona	1509029-01	1
Eu Rho/gehe	Hidrocortisona	1611016-01	1
EuRho / Noweda	Hidrocortisona	1906033-01	1
EuRho 12.03.2013 Anzag	Hidrocortisona	1112030-01	1
EuRho/ Anzag	Hidrocortisona	113(1906033-01)	1
Eurho/ Phönix	Hidrocortisona	180200901	1
EuRho/AHD	Hidrocortisona	1802009-01	1
EuRho/GEHE	Hidrocortisona	1611016-01	1
EuRho/Jenne	Hidrocortisona	1906033-01	1
EuRho/Noweda	Hidrocortisona	1611016-01	1
Eurho/Phönix	Hidrocortisona	210100302	1
EuRho	Hidrocortisona	1107005-02	1
EuRho	Hidrocortisona	1202032-01	1
EuRho	Hidrocortisona	1204037-01	1
EuRho	Hidrocortisona	1405001-01	3
EuRho	Hidrocortisona	1509029-01	1
EuRho	Hidrocortisona	1611016-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Hidrocortisona	180200-01	1
EuRho	Hidrocortisona	2101003-01	1
Euro / AHD	Hidrocortisona	1906033-01	1
EURO / Gehe	Hidrocortisona	1405001-01	1
Euro Gehe	Hidrocortisona	1611016-01	1
Euro Gehe	Hidrocortisona	1802009-01	1
Euro OT/Anzag	Hidrocortisona	1611016-01	3
Euro OTC	Hidrocortisona	100(1906033-01)	1
Euro OTC	Hidrocortisona	101(1906033-01)	1
Euro OTC	Hidrocortisona	102(1906033-01)	1
Euro OTC	Hidrocortisona	103(1906033-01)	1
Euro OTC	Hidrocortisona	104(1906033)	1
Euro OTC	Hidrocortisona	105(1906033-01)	1
Euro OTC	Hidrocortisona	106(1906033-01)	1
Euro OTC	Hidrocortisona	107(1906033-01)	1
Euro OTC	Hidrocortisona	108(1906033-01)	1
Euro OTC	Hidrocortisona	1082009-01	1
Euro OTC	Hidrocortisona	109(1906033-01)	1
Euro OTC	Hidrocortisona	1096033-01	1
Euro OTC	Hidrocortisona	110(1906033-01)	1
Euro OTC	Hidrocortisona	1107005-01	1
Euro OTC	Hidrocortisona	1107005-02	3
Euro OTC	Hidrocortisona	1107005-03	8
Euro OTC	Hidrocortisona	111(1906033-01)	1
Euro OTC	Hidrocortisona	1112030-01	9
Euro OTC	Hidrocortisona	112(1906033-01)	1
Euro OTC	Hidrocortisona	11611016-01	1
Euro OTC	Hidrocortisona	119(2101003-01)	1
Euro OTC	Hidrocortisona	1202032-01	3
Euro OTC	Hidrocortisona	120403701	3
Euro OTC	Hidrocortisona	1204037-01	26
Euro OTC	Hidrocortisona	1204307-01	1
Euro OTC	Hidrocortisona	12060018-01	1
Euro OTC	Hidrocortisona	1206018-01	23
Euro OTC	Hidrocortisona	120618-01	1
Euro OTC	Hidrocortisona	1405001	1
Euro OTC	Hidrocortisona	1405001-01	2
Euro OTC	Hidrocortisona	1408023-01	4
Euro OTC	Hidrocortisona	1501034	1
Euro OTC	Hidrocortisona	1501034-01	10
Euro OTC	Hidrocortisona	1505010601	1
Euro OTC	Hidrocortisona	150501601	1
Euro OTC	Hidrocortisona	1505016-01	30
Euro OTC	Hidrocortisona	15050-16-01	1
Euro OTC	Hidrocortisona	150516-01	1
Euro OTC	Hidrocortisona	150902	1
Euro OTC	Hidrocortisona	1509029	1
Euro OTC	Hidrocortisona	150902901	2
Euro OTC	Hidrocortisona	1509029-01	42
Euro OTC	Hidrocortisona	150929-01	1
Euro OTC	Hidrocortisona	15278703	1
Euro OTC	Hidrocortisona	157015	2
Euro OTC	Hidrocortisona	16004612	1
Euro OTC	Hidrocortisona	161016-01	1
Euro OTC	Hidrocortisona	16110016-01	1
Euro OTC	Hidrocortisona	1611016	1
Euro OTC	Hidrocortisona	161101601	3
Euro OTC	Hidrocortisona	1611016-01	75
Euro OTC	Hidrocortisona	161116-01	1
Euro OTC	Hidrocortisona	16272305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Hidrocortisona	16272311	1
Euro OTC	Hidrocortisona	1708006-01	1
Euro OTC	Hidrocortisona	17119402	1
Euro OTC	Hidrocortisona	17119403	2
Euro OTC	Hidrocortisona	17256603	1
Euro OTC	Hidrocortisona	17351202	1
Euro OTC	Hidrocortisona	1801009-01	1
Euro OTC	Hidrocortisona	1802008-01	1
Euro OTC	Hidrocortisona	1802009	1
Euro OTC	Hidrocortisona	180200901	4
Euro OTC	Hidrocortisona	1802009-01	84
Euro OTC	Hidrocortisona	18091501	1
Euro OTC	Hidrocortisona	18091506	1
Euro OTC	Hidrocortisona	181102182	1
Euro OTC	Hidrocortisona	1906033	2
Euro OTC	Hidrocortisona	190603301	1
Euro OTC	Hidrocortisona	1906033-01	91
Euro OTC	Hidrocortisona	190633-01	3
Euro OTC	Hidrocortisona	19069033-01	1
Euro OTC	Hidrocortisona	2019Q-01719	1
Euro OTC	Hidrocortisona	2101003-001	1
Euro OTC	Hidrocortisona	210100301	1
Euro OTC	Hidrocortisona	2101003-01	49
Euro OTC	Hidrocortisona	2101003-02	8
Euro OTC	Hidrocortisona	210818A	1
Euro OTC	Hidrocortisona	210826	1
Euro OTC	Hidrocortisona	210906(2101003-01)	1
Euro OTC	Hidrocortisona	211118(2101003-01)	1
Euro OTC	Hidrocortisona	2205003-01	5
Euro OTC	Hidrocortisona	29011504	1
Euro OTC	Hidrocortisona	3817A-01719	1
Euro OTC	Hidrocortisona	4091510	1
Euro OTC	Hidrocortisona	4112A-01719	1
Euro OTC	Hidrocortisona	4616U-01719	1
Euro OTC	Hidrocortisona	6051502	1
Euro OTC	Hidrocortisona	715Q-01719	1
Euro OTC	Hidrocortisona	79(1802009-01)	1
Euro OTC	Hidrocortisona	80(1802009-01)	1
Euro OTC	Hidrocortisona	81(1802009-01)	1
Euro OTC	Hidrocortisona	82(1802009-01)	1
Euro OTC	Hidrocortisona	8639285	1
Euro OTC	Hidrocortisona	906033-01	1
Euro OTC	Hidrocortisona	K05B20160909	1
Euro OTC	Hidrocortisona	K05B20180323	1
Euro OTC	Hidrocortisona	K05M20170313	1
Euro OTC	Hidrocortisona	k05m20201110	1
Euro OTC	Hidrocortisona	L39844	1
Euro/ Phönix	Hidrocortisona	1509029-01	1
Euro/Phönix	Hidrocortisona	210100301	1
Euro/Sanacorp	Hidrocortisona	1906033-01	2
Fagro/Otto Geilenkirchen	Hidrocortisona	19k05-b02-195614	1
Fagron	Hidrocortisona		2
Fagron	Hidrocortisona	11021403	1
Fagron	Hidrocortisona	114(19K05-B02-195615)	1
Fagron	Hidrocortisona	115(19K015-0004)	1
Fagron	Hidrocortisona	116(19K05-B02-195615)	1
Fagron	Hidrocortisona	117(19K05-B02-195615)	1
Fagron	Hidrocortisona	11K18-N01	2
Fagron	Hidrocortisona	12/25-N01	1
Fagron	Hidrocortisona	1204037-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hidrocortisona	120601801	1
Fagron	Hidrocortisona	12091401	1
Fagron	Hidrocortisona	12104304	1
Fagron	Hidrocortisona	12119303	1
Fagron	Hidrocortisona	12G19-N01	2
Fagron	Hidrocortisona	12I25-N01	2
Fagron	Hidrocortisona	13341510	1
Fagron	Hidrocortisona	13H08-B01-285469	1
Fagron	Hidrocortisona	13H08-B01-285472	1
Fagron	Hidrocortisona	13H08B01285473	1
Fagron	Hidrocortisona	13H08-B01-285473	1
Fagron	Hidrocortisona	13H08-B01-28571	1
Fagron	Hidrocortisona	13K22-B01-288282	1
Fagron	Hidrocortisona	13K22-B01-288283	1
Fagron	Hidrocortisona	13K22-B01-288284	3
Fagron	Hidrocortisona	14/05-B02-300227	2
Fagron	Hidrocortisona	14/05-BO2-300227	1
Fagron	Hidrocortisona	14B04-B02	2
Fagron	Hidrocortisona	14B04-B02-293422	3
Fagron	Hidrocortisona	14B04-B02-293423	4
Fagron	Hidrocortisona	14B04-B02-293424	6
Fagron	Hidrocortisona	14I05-B02	2
Fagron	Hidrocortisona	14I05-B02-300227	1
Fagron	Hidrocortisona	14I05-B02-300228	1
Fagron	Hidrocortisona	14I05-B02-300229	1
Fagron	Hidrocortisona	14l05-B02-300227	1
Fagron	Hidrocortisona	14l05-B02-300228	1
Fagron	Hidrocortisona	15/25-B01-313084	1
Fagron	Hidrocortisona	15/25-B01-318727	1
Fagron	Hidrocortisona	15015	1
Fagron	Hidrocortisona	1509029-01	1
Fagron	Hidrocortisona	15D14-B02	1
Fagron	Hidrocortisona	15D14-B02-311696	5
Fagron	Hidrocortisona	15I04-B03-315021	1
Fagron	Hidrocortisona	15I25-B01-318727	1
Fagron	Hidrocortisona	15l25-B01-318486	1
Fagron	Hidrocortisona	16272311	1
Fagron	Hidrocortisona	16A19-B06	1
Fagron	Hidrocortisona	16A19-B06-320970	20
Fagron	Hidrocortisona	16A19-B06-321981	2
Fagron	Hidrocortisona	16A19-B06-321982	1
Fagron	Hidrocortisona	16H01-B01	1
Fagron	Hidrocortisona	16H01-B01-324891	1
Fagron	Hidrocortisona	16H01-B01-324944	5
Fagron	Hidrocortisona	16H01-B01-326071	3
Fagron	Hidrocortisona	16J26-B04	1
Fagron	Hidrocortisona	16J26-B04-328188	1
Fagron	Hidrocortisona	16J26-B04-329419	1
Fagron	Hidrocortisona	16j26-b04-330339	1
Fagron	Hidrocortisona	16J26-B04-330340	2
Fagron	Hidrocortisona	17/12-b05-344220	1
Fagron	Hidrocortisona	17/12-B05-344220	2
Fagron	Hidrocortisona	17/12-B05-345540	1
Fagron	Hidrocortisona	17/12-Bos-344220	1
Fagron	Hidrocortisona	17119405	1
Fagron	Hidrocortisona	17-12B05-342611	1
Fagron	Hidrocortisona	1712-B05-345540	2
Fagron	Hidrocortisona	17256604	1
Fagron	Hidrocortisona	17351205	1
Fagron	Hidrocortisona	17c13-B06	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hidrocortisona	17C13-B06	1
Fagron	Hidrocortisona	17C13-B06-333045	4
Fagron	Hidrocortisona	17E10-B04	2
Fagron	Hidrocortisona	17E10-B04-334857	5
Fagron	Hidrocortisona	17E-10-B04-334857	1
Fagron	Hidrocortisona	17E10-B04-334858	4
Fagron	Hidrocortisona	17e10-b04-335056	1
Fagron	Hidrocortisona	17E10-B04-335056	3
Fagron	Hidrocortisona	17E10B04335656	1
Fagron	Hidrocortisona	17E10-B04-335656	2
Fagron	Hidrocortisona	17E10-B04-336435	7
Fagron	Hidrocortisona	17E10-B04-336436	2
Fagron	Hidrocortisona	17g25-b02-340864	1
Fagron	Hidrocortisona	17G25-B02-340864	2
Fagron	Hidrocortisona	17G25-B02-340865	1
Fagron	Hidrocortisona	17I12-B05	1
Fagron	Hidrocortisona	17I12-B05-344220	2
Fagron	Hidrocortisona	17I12-B05-34554	1
Fagron	Hidrocortisona	18091501	1
Fagron	Hidrocortisona	18B21-B07	2
Fagron	Hidrocortisona	18B21-B07-348430	3
Fagron	Hidrocortisona	18B21-B07-348431	4
Fagron	Hidrocortisona	18B21-B07-348432	3
Fagron	Hidrocortisona	18B21-B07-360920	1
Fagron	Hidrocortisona	19051403	1
Fagron	Hidrocortisona	19K05-802-195615	1
Fagron	Hidrocortisona	19K05-B02-195613	3
Fagron	Hidrocortisona	19K05-B02-195614	3
Fagron	Hidrocortisona	19k05-b02-195615	1
Fagron	Hidrocortisona	19K05-B02-195615	6
Fagron	Hidrocortisona	20B17-802-2000542	1
Fagron	Hidrocortisona	20B17-B02-200514	4
Fagron	Hidrocortisona	20B17-B02-200543	4
Fagron	Hidrocortisona	20B17-B02-200544	8
Fagron	Hidrocortisona	20B17-B02-200571	2
Fagron	Hidrocortisona	21011003-02	1
Fagron	Hidrocortisona	-21965000	1
Fagron	Hidrocortisona	22E09-B02-219650	1
Fagron	Hidrocortisona	23D06-B02-234497	1
Fagron	Hidrocortisona	20B17-B02-200543	1
Fagron	Hidrocortisona	5061304	1
Fagron	Hidrocortisona	B0-20051004	1
Fagron	Hidrocortisona	B02-2005104	1
Fagron	Hidrocortisona	B02-2005403	3
Fagron	Hidrocortisona	BO2-1956104	1
Fagron	Hidrocortisona	K05B20130407M	1
Fagron	Hidrocortisona	K05B20131101	1
Fagron	Hidrocortisona	K05M20170702	1
Fagron	Hidrocortisona	PH132	1
Fagron	Hidrocortisona	T3319	1
Fargo/Anzag	Hidrocortisona	17E10-B04-335056	1
Fargon	Hidrocortisona	17E10-B04-334858	1
fargon	Hidrocortisona	T3325	1
fargron	Hidrocortisona	13K22-B01-288284	1
Fiebig	Hidrocortisona	1509029-01	2
Fiebig	Hidrocortisona	16095207	1
Fiebig	Hidrocortisona	16095210	1
Fiebig	Hidrocortisona	17119402	2
Fiebig	Hidrocortisona	17256602	1
Fiebig	Hidrocortisona	18091520	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Hidrocortisona	18091525	1
Fiebig	Hidrocortisona	18091528	1
Finteler Apotheke	Hidrocortisona	1611016-01	3
Fischar/ Anzag	Hidrocortisona	118(20B17-B02-200544)	1
Fragon/Anzag	Hidrocortisona	19K05-b02-195615	1
Fragon/Sanacorp	Hidrocortisona	17E10-B04-335056	1
Gatt-Koller	Hidrocortisona	1804169	1
Gatt-Koller	Hidrocortisona	20172187	1
Gatt-Koller	Hidrocortisona	22J00274	1
GEHE 03.05.2014	Hidrocortisona	13155605	1
GEHE 14.04.2014	Hidrocortisona	13069509	1
Gehe,27.0415	Hidrocortisona	14301310	1
Gehe/EuRho	Hidrocortisona	19060033-01	1
Gehe/Europharm	Hidrocortisona	1802009-01	1
Gehe/Jenne	Hidrocortisona	20004116001	1
Gehe	Hidrocortisona	1206018-01	2
Gehe	Hidrocortisona	12104304	3
Gehe	Hidrocortisona	13069510	1
Gehe	Hidrocortisona	13341510	1
Gehe	Hidrocortisona	13H08-B01-285469	1
Gehe	Hidrocortisona	13H08-B01-285471	1
Gehe	Hidrocortisona	1405001-01	1
Gehe	Hidrocortisona	1501034-01	1
Gehe	Hidrocortisona	1509029-01	1
Gehe	Hidrocortisona	1611016-01	1
gehe	Hidrocortisona	16255607	1
Gehe	Hidrocortisona	16255607	1
Gehe	Hidrocortisona	16255608	1
Gehe	Hidrocortisona	16272306	1
GEHE	Hidrocortisona	16272311	1
Gehe	Hidrocortisona	17256604	1
Gehe	Hidrocortisona	17351203	1
Gehe	Hidrocortisona	17351206	1
Gehe	Hidrocortisona	17E10-B04-335656	1
Gehe	Hidrocortisona	1802009-01	1
Gehe	Hidrocortisona	18091502	2
Gehe	Hidrocortisona	18091521	1
Gehe	Hidrocortisona	183243004	1
Gehe	Hidrocortisona	18324301	2
GEHE	Hidrocortisona	18324301	1
Gehe	Hidrocortisona	18324303	1
Gehe	Hidrocortisona	18324310	1
Gehe	Hidrocortisona	1906033-01	1
Gehe	Hidrocortisona	192241002	1
Gehe	Hidrocortisona	2004116006	1
Gehe	Hidrocortisona	21001215003	1
Gehe	Hidrocortisona	21001215013	1
Gehe	Hidrocortisona	21001215019	1
Gehe	Hidrocortisona	21001215021	1
Gehe	Hidrocortisona	21001215027	2
Gehe	Hidrocortisona	21001215035	3
Gehe	Hidrocortisona	2101003-01	1
Gehe	Hidrocortisona	22003779004	1
GEHE	Hidrocortisona	2205003-01	1
Ge-Hh	Hidrocortisona	192241002	1
Geilenkirchen	Hidrocortisona	1611016-01	1
Geilenkirchen	Hidrocortisona	20004116007	1
Henan Lihua Pharm/AHD	Hidrocortisona	18B21-B07-348430	1
Henan Lihua Pharmace...	Hidrocortisona	1906033-01	1
Henan/Noweda	Hidrocortisona	K05M20170408	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Henan/Noweda	Hidrocortisona	K05M20170701	1
Jenne	Hidrocortisona	18324307	2
Jenne	Hidrocortisona	22003779004	1
Jenne	Hidrocortisona	22003779005	1
Kehr	Hidrocortisona	16095213	1
Kehr	Hidrocortisona	17119407	1
Kehr	Hidrocortisona	17256602	1
Kehr	Hidrocortisona	20004116003	2
Kehr	Hidrocortisona	21001215026	2
Kehr	Hidrocortisona	21001215027	2
Kehr	Hidrocortisona	21001215029	1
Kehr	Hidrocortisona	22003779004	2
Kehr	Hidrocortisona	2205003-01	2
Klenk	Hidrocortisona	12167007	1
L10	Hidrocortisona	16H01-B01-326071	2
L12	Hidrocortisona	1802009-01	1
Laborchemie Apolda/Phönix	Hidrocortisona	15181004	1
Midas	Hidrocortisona	17256602	1
Midas	Hidrocortisona	18091519	1
Nachprüfung 2312	Hidrocortisona	10282201	1
Nachprüfung	Hidrocortisona	123456	1
Nachprüfung	Hidrocortisona	2082019-6	1
Noweda 28.10.2019	Hidrocortisona	18091531	1
Noweda 5,45 06.0...	Hidrocortisona	18324311	1
Noweda 5,45 14.04.2020	Hidrocortisona	183243002	1
Noweda Herford	Hidrocortisona	21001215006	1
Noweda/ Caesar&Loren...	Hidrocortisona	18324303	1
Noweda	Hidrocortisona	12104303	1
Noweda	Hidrocortisona	12167001	1
Noweda	Hidrocortisona	13155605	1
Noweda	Hidrocortisona	16004612	1
Noweda	Hidrocortisona	16095212	1
Noweda	Hidrocortisona	1611016-01	1
Noweda	Hidrocortisona	16255608	1
Noweda	Hidrocortisona	17090005	1
Noweda	Hidrocortisona	17119402	1
Noweda	Hidrocortisona	17256602	3
Noweda	Hidrocortisona	17256605	2
Noweda	Hidrocortisona	17351203	1
Noweda	Hidrocortisona	17351204	1
Noweda	Hidrocortisona	17351210	1
noweda	Hidrocortisona	18091506	1
Noweda	Hidrocortisona	183243002	2
Noweda	Hidrocortisona	18324301	1
Noweda	Hidrocortisona	18324308	1
Noweda	Hidrocortisona	18324311	1
Noweda	Hidrocortisona	192241005	1
Noweda	Hidrocortisona	192241008	1
Noweda	Hidrocortisona	20004116004	1
Noweda	Hidrocortisona	20004116005	2
Noweda	Hidrocortisona	20004116007	1
Noweda	Hidrocortisona	21001215003	4
Noweda	Hidrocortisona	22003779004	1
Noweda	Hidrocortisona	22003779006	2
NOWEDA	Hidrocortisona	22003779006	1
Otto Geilenkirchen	Hidrocortisona	21001215029	1
Pharmachem/ Anzag	Hidrocortisona	18091520	1
Pharmacia&Upjohn/ Phönix	Hidrocortisona	13155614	1
Phoenix	Hidrocortisona	13341504	1
Phoenix	Hidrocortisona	1509029-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Hidrocortisona	16095207	1
Phoenix	Hidrocortisona	1611016-01	1
Phoenix	Hidrocortisona	17119405	3
Phoenix	Hidrocortisona	17256605	1
Phoenix	Hidrocortisona	18091528	1
Phoenix	Hidrocortisona	18091531	1
Phoenix	Hidrocortisona	183243002	1
Phoenix	Hidrocortisona	18324301	1
Phoenix	Hidrocortisona	18324306	1
Phoenix	Hidrocortisona	18324311	1
phoenix	Hidrocortisona	192241008	1
Phoenix	Hidrocortisona	21001215005	1
Phoenix	Hidrocortisona	21001215029	1
Phoenix	Hidrocortisona	2101003-01	2
Phoenix	Hidrocortisona	3117	1
Phoenix	Hidrocortisona	3370	1
Phönix 15.7.2019	Hidrocortisona	18091520	1
Phönix Caesar u. Loretz	Hidrocortisona	13225507	1
Phönix Gotha	Hidrocortisona	12104309	1
Phönix Gotha	Hidrocortisona	13341502	1
Phönix Gotha	Hidrocortisona	15021107	1
Phönix Gotha	Hidrocortisona	15181004	1
Phönix Gotha	Hidrocortisona	18324307	1
Phönix, Caesar&Loret…	Hidrocortisona	183243003	1
phönix	Hidrocortisona		2
Phönix	Hidrocortisona	11119-N03	1
Phönix	Hidrocortisona	1204037-01	1
Phönix	Hidrocortisona	12167001	2
Phönix	Hidrocortisona	12167010	1
Phönix	Hidrocortisona	13341504	2
Phönix	Hidrocortisona	13341508	1
Phönix	Hidrocortisona	1408023-01	1
phönix	Hidrocortisona	14301306	1
Phönix	Hidrocortisona	15181005	1
phönix	Hidrocortisona	15181013	1
Phönix	Hidrocortisona	1611016-01	2
Phönix	Hidrocortisona	16110161-01	1
Phönix	Hidrocortisona	16272306	1
Phönix	Hidrocortisona	17119406	1
PHÖNIX	Hidrocortisona	17119410	1
Phönix	Hidrocortisona	17256602	1
Phönix	Hidrocortisona	17256603	1
Phönix	Hidrocortisona	17351206	2
Phönix	Hidrocortisona	17E10-B04-334858	1
Phönix	Hidrocortisona	1802009-01	3
Phönix	Hidrocortisona	18081508	1
Phönix	Hidrocortisona	18091505	1
Phönix	Hidrocortisona	1824302	1
Phönix	Hidrocortisona	183243006	1
Phönix	Hidrocortisona	18324302	1
Phönix	Hidrocortisona	18B21-B07-360920	1
Phönix	Hidrocortisona	1906033	1
Phönix	Hidrocortisona	1906033-01	3
PHÖNIX	Hidrocortisona	192241008	1
Phönix	Hidrocortisona	20004116002	1
Phönix	Hidrocortisona	20004116007	1
Phönix	Hidrocortisona	201073010	1
Phönix	Hidrocortisona	21001215005	3
Phönix	Hidrocortisona	21001215007	1
Phönix	Hidrocortisona	21001215032	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Hidrocortisona	2101003-01	2
Phönix	Hidrocortisona	22003779012	1
Phönix	Hidrocortisona	3181	1
Phönix	Hidrocortisona	Hy19	1
Röntgen	Hidrocortisona	17256605	1
Röntgen	Hidrocortisona	1906033-01	1
sana corp	Hidrocortisona	13069507	1
Sana	Hidrocortisona	18091524	3
Sanacorp	Hidrocortisona	1112030-01	1
Sanacorp	Hidrocortisona	13069509	1
Sanacorp	Hidrocortisona	13341509	1
Sanacorp	Hidrocortisona	14301307	1
Sanacorp	Hidrocortisona	14B04-B02	1
Sanacorp	Hidrocortisona	1509029-01	1
sanacorp	Hidrocortisona	15181012	1
sanacorp	Hidrocortisona	15181013	1
Sanacorp	Hidrocortisona	16004607	1
Sanacorp	Hidrocortisona	17256604	1
Sanacorp	Hidrocortisona	1802009-01	3
Sanacorp	Hidrocortisona	18091501	1
Sanacorp	Hidrocortisona	18091507	1
Sanacorp	Hidrocortisona	18091520	1
Sanacorp	Hidrocortisona	183243006	1
Sanacorp	Hidrocortisona	1906033-01	1
sanacorp	Hidrocortisona	192241008	1
Sanacorp	Hidrocortisona	192241008	3
Sanacorp	Hidrocortisona	20b17-b02-200514	1
Sanacorp	Hidrocortisona	21001215014	1
Sanacorp	Hidrocortisona	21001215023	2
Sanacorp	Hidrocortisona	22003779004	2
Sanacorp	Hidrocortisona	42/AKD6	1
Sanacorp	Hidrocortisona	Fagron	1
Sanacorp	Hidrocortisona	K05M20221003	1
Spangro 22.05.2014	Hidrocortisona	13341504	2
Spangro 23.1.2014	Hidrocortisona	13069510	1
Spangro_21.05.2019	Hidrocortisona	18091524	1
Tianjin JP / Gehe	Hidrocortisona	183243004	1
Tianjin/Noweda	Hidrocortisona	T3307	1
Tianjin/Noweda	Hidrocortisona	TA0075	1
Upjohn/Phönix	Hidrocortisona	1509029-01	1
VDL	Hidrocortisona	18091525	1
xxx	Hidrocortisona	911Q-01719	2

- 231 571 spectra from 1514 *Apo-Ident* customers from a total of 48 711 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hidrocortisona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidrocortisona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	661	0	152 301
Type B	0	1119	0	200 965
Type C	0	4487	9	231 571

The substance/substance group *Hidrocortisona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4638 %)
Type C	100.0000 % (> 99.9007 %)	99.7998 % (> 99.7331 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21293	21899	7,22	116,60
21461	21899	8,00	117,12
21463	21899	3,34	117,05
21899	21899	0,00	117,25
22829	22838	7,67	119,75
22837	22838	5,18	117,60
22838	22838	0,00	119,73
22910	22910	0,00	120,10
22928	22910	5,74	122,00
24020	24020	0,00	119,55
25571	25571	0,00	122,58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidroquinona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20091-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidroquinona; Hydrochinonum

Special notes

When selecting the *Hidroquinona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidroquinona	8	4	82

Second-stage model

For differentiation of the substance/substance group *Hidroquinona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidroquinona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Resorcinol	44,48	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidroquinona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidroquinona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidroquinona	12288505	20884	40	20121015
Caelo	Hidroquinona	14026904	21468	60	20140122
Caelo	Hidroquinona	14281501	21791	60	AR-15-FG-008058-01
Caelo	Hidroquinona	14280110	21923	60	20141017
Caelo	Hidroquinona	15057001	22324	60	20150306
Caelo	Hidroquinona	15057001	22351	60	20150306
Caelo	Hidroquinona	182306	24761	40	20181008*
Caelo	Hidroquinona	192642	24890	40	20191115*
Gatt-Koller	Hidroquinona	23J02483	27097	30	20240109
Gatt-Koller	Hidroquinona	23J02483	27097SI	20	20240109

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 470 spectra of 10 reference samples from the substance/substance group *Hidroquinona*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 492 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 5 reference samples from the substance/substance group *Hidroquinona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidroquinona	15057004	21975	60
Caelo	Hidroquinona	16023105	23114	40
Caelo	Hidroquinona	172215	23654	40
Caelo	Hidroquinona	23000425	27226	40
Caelo	Hidroquinona	23000425	27226SI	20

- 201 884 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 524 spectra from 337 *Apo-Ident* customers from 90 batches from the substance/substance group *Hidroquinona*.

- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hidroquinona	20001617007	2
	Hidroquinona	21003639007	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Hidroquinona	21003639008	1
	Hidroquinona	21003639010	3
	Hidroquinona	21003639011	5
14026902	Hidroquinona	InterneCharge1214Q	1
16023112	Hidroquinona	16023112	1
A.H. 14.06.13 ek: 3,97EUR	Hidroquinona	12288505	1
ACM	Hidroquinona	KNC0635J17	1
ACM	Hidroquinona	KNC1047J15	2
AHD	Hidroquinona	13105405	1
AHD	Hidroquinona	21003639010	1
AHL	Hidroquinona	16023102	1
Alli	Hidroquinona	21003639010	1
Alliance Healthcare	Hidroquinona	20001617007	1
Allianz	Hidroquinona	16023116	1
Anzag	Hidroquinona	12156705	1
apomix	Hidroquinona	13105408	1
Caelo	Hidroquinona		3
Caelo	Hidroquinona	1(192642008)0	1
Caelo	Hidroquinona	10145101	1
Caelo	Hidroquinona	10145103	1
Caelo	Hidroquinona	10145113	2
Caelo	Hidroquinona	11163905	5
Caelo	Hidroquinona	11163907	5
Caelo	Hidroquinona	11163912	4
Caelo	Hidroquinona	11163912/Int312052	1
Caelo	Hidroquinona	1163902	1
Caelo	Hidroquinona	12156703	1
Caelo	Hidroquinona	12156705	5
Caelo	Hidroquinona	12156706	1
Caelo	Hidroquinona	1228503	1
Caelo	Hidroquinona	12288502	2
Caelo	Hidroquinona	12288503	2
Caelo	Hidroquinona	12288505	13
Caelo	Hidroquinona	1263912	1
Caelo	Hidroquinona	13105402	5
Caelo	Hidroquinona	13105405	6
Caelo	Hidroquinona	13105408	7
Caelo	Hidroquinona	14026902	5
Caelo	Hidroquinona	14026904	1
Caelo	Hidroquinona	1410401	1
Caelo	Hidroquinona	14121202	1
Caelo	Hidroquinona	14180401	4
Caelo	Hidroquinona	14180406	3
Caelo	Hidroquinona	14180410	4
Caelo	Hidroquinona	14280104	5
Caelo	Hidroquinona	14280105	2
Caelo	Hidroquinona	14281501	11
Caelo	Hidroquinona	14281504	1
Caelo	Hidroquinona	14281507	4
Caelo	Hidroquinona	15023105	1
Caelo	Hidroquinona	15057001	11
Caelo	Hidroquinona	15057002	1
Caelo	Hidroquinona	15057004	13
Caelo	Hidroquinona	15057010	17
Caelo	Hidroquinona	160123118	1
Caelo	Hidroquinona	160223105	1
Caelo	Hidroquinona	16023102	3
Caelo	Hidroquinona	16023105	16
Caelo	Hidroquinona	16023112	11
Caelo	Hidroquinona	16023113	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidroquinona	160231135430	1
Caelo	Hidroquinona	16023116	25
Caelo	Hidroquinona	16023118	16
Caelo	Hidroquinona	16023118P-190314-1	1
Caelo	Hidroquinona	16051502	1
Caelo	Hidroquinona	17221503	1
Caelo	Hidroquinona	17221508	10
Caelo	Hidroquinona	18017902	28
Caelo	Hidroquinona	18017905	9
Caelo	Hidroquinona	1801792	1
Caelo	Hidroquinona	18031403	1
Caelo	Hidroquinona	18230602	15
Caelo	Hidroquinona	18230607	10
Caelo	Hidroquinona	192642003	26
Caelo	Hidroquinona	192642008	4
Caelo	Hidroquinona	20001617002	10
Caelo	Hidroquinona	20001617004	1
Caelo	Hidroquinona	20001617005	6
Caelo	Hidroquinona	20001617007	18
Caelo	Hidroquinona	2000167007	1
Caelo	Hidroquinona	20101806	1
Caelo	Hidroquinona	20200712-3	1
Caelo	Hidroquinona	21003639007	3
Caelo	Hidroquinona	21003639010	1
Caelo	Hidroquinona	21102014A	1
Caelo	Hidroquinona	3281	1
Caelo	Hidroquinona	4017A-01717	1
Caelo	Hidroquinona	52840166	1
Caelo	Hidroquinona	8725	1
Caelo	Hidroquinona	8816-10-583	1
Caeolo/Gehe	Hidroquinona	16023116	1
Caeolo	Hidroquinona	16023105	1
Caesar & Loretz GmbH...	Hidroquinona	18017902	1
Caesar & Loretz GmbH...	Hidroquinona	192642003	1
Caesar & Loretz GmbH...	Hidroquinona	11163912	1
Caesar & Loretz GmbH...	Hidroquinona	18017902	1
Caesar & Loretz GmbH...	Hidroquinona	20001617002	1
Caesar & Loretz GmbH...	Hidroquinona	18230607	1
Caesar & Loretz GmbH...	Hidroquinona	20001617007	1
Caesar & Loretz GmbH...	Hidroquinona	192642003	1
Caesar & Loretz GmbH...	Hidroquinona	20001617002	1
Caesar & Loretz GmbH...	Hidroquinona	20001617002	1
Caesar & Loretz GmbH	Hidroquinona	13105405	1
Caesar & Loretz GmbH	Hidroquinona	16023105	1
Caesar & Loretz GmbH	Hidroquinona	18017902	3
Caesar & Loretz GmbH	Hidroquinona	18230602	4
Caesar & Loretz GmbH	Hidroquinona	18230607	1
Caesar & Loretz GmbH	Hidroquinona	192642003	8
Caesar & Loretz GmbH	Hidroquinona	192642008	2
Caesar & Loretz GmbH	Hidroquinona	20001617002	6
Caesar & Loretz GmbH	Hidroquinona	20001617005	2
Caesar & Loretz GmbH	Hidroquinona	20001617006	1
Caesar & Loretz GmbH	Hidroquinona	20001617007	9
Caesar & Loretz GmbH	Hidroquinona	21003639002	1
Caesar & Loretz GmbH	Hidroquinona	21003639007	2
Caesar & Loretz GmbH	Hidroquinona	21003639010	2
Caesar & Loretz Hilden	Hidroquinona	20001617002	1
Caesar & Loretz	Hidroquinona	16023112	1
Caesar & Loretz	Hidroquinona	192642008	1
Caesar / Gehe	Hidroquinona	16023116	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar und Loretz	Hidroquinona	18230607	1
Cealo	Hidroquinona	192642003	1
Cesar&Loretz GmbH	Hidroquinona	192642008	1
E Plus	Hidroquinona	18017902	1
Euro OTC	Hidroquinona	16023118	2
Euro/Sanacorp	Hidroquinona	15057004	1
Fagron	Hidroquinona		1
Fiebig	Hidroquinona	16023116	1
Gatt-Koller	Hidroquinona	1803302	4
Gatt-Koller	Hidroquinona	22J00202	1
Gehe/Gehe	Hidroquinona	14280110	1
Gehe	Hidroquinona	12156706	2
GEHE	Hidroquinona	16023105	1
GEHE	Hidroquinona	16023118	1
GEHE	Hidroquinona	18017902	1
Gehe	Hidroquinona	21003639007	2
Gehe	Hidroquinona	21003639010	1
Kehr	Hidroquinona	16023112	1
Kehr	Hidroquinona	16023113	1
Noweda	Hidroquinona	16023116	2
noweda	Hidroquinona	18230602	1
Noweda	Hidroquinona	21003639010	1
Phoenix Goettin	Hidroquinona	14281501	1
Phoenix	Hidroquinona	16023105	1
Phoenix	Hidroquinona	18017905	1
Phoenix	Hidroquinona	18230602	1
Phoenix	Hidroquinona	192642003	1
Phoenix	Hidroquinona	200671007	1
Phönix	Hidroquinona	12288503	2
Phönix	Hidroquinona	13105408	1
phönix	Hidroquinona	16023105	1
Sanacorp	Hidroquinona	12156703	1
Sanacorp	Hidroquinona	12288503	1
Sanacorp	Hidroquinona	16023103	1
Sanacorp	Hidroquinona	16023118	1
Sanacorp	Hidroquinona	18230602	1
Sanacorp	Hidroquinona	18230607	1
Sanacorp	Hidroquinona	21003639007	1
Sanacorp	Hidroquinona	23000425005	1
Sanacorp	Hidroquinona	5118M-01717	1

- 235 543 spectra from 1515 *Apo-Ident* customers from a total of 49 170 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hidroquinona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidroquinona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	470	0	152 492
Type B	0	200	0	201 884
Type C	0	505	19	235 543

The substance/substance group *Hidroquinona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7234 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	96.3740 % (> 95.8015 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20884	21791	3,62	64,66
21468	21791	11,38	62,44
21791	21791	0,00	62,27
21923	21791	5,55	62,32
22324	21791	5,03	60,77
22351	21791	3,89	60,76
24761	24761	0,00	62,02
24890	24890	0,00	63,08
27097	21791	15,52	70,20

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidroxietilcelulose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006129-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidroxietilcelulose; Hydroxyethylcellulosum

Special notes

When selecting the *Hidroxietilcelulose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidroxietilcelulose	9	38	0

Second-stage model

For differentiation of the substance/substance group *Hidroxietilcelulose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidroxietilcelulose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	88,51	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidroxietilcelulose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidroxietilcelulose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidroxietilcelulose	181131	26775	40	20180612*
Caelo	Hidroxietilcelulose	22002812	26779	40	20221031*
Caelo	Hidroxietilcelulose	22002812	26779SI	20	20221031*
Caelo	Hidroxietilcelulose	23000202	26781	40	20230210*
Caelo	Hidroxietilcelulose	23000202	26781SI	20	20230210*
Caelo	Hidroxietilcelulose	13378506	26785	40	1507205
Caelo	Hidroxietilcelulose	12274720	26789	20	20121001
Caelo	Hidroxietilcelulose	171151	26793	40	20170523*
Caelo	Hidroxietilcelulose	22000306	26812	40	20220314*
Euro OTC	Hidroxietilcelulose	2306013	26884	40	20230801*
Euro OTC	Hidroxietilcelulose	2408008	27390	40	20241008*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 11 reference samples from the substance/substance group *Hidroxietilcelulose*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 582 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1710 spectra of 45 reference samples from the substance/substance group *Hidroxietilcelulose*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidroxietilcelulose	190174	26774	40
Caelo	Hidroxietilcelulose	191675	26776	40
Caelo	Hidroxietilcelulose	20000136	26777	40
Caelo	Hidroxietilcelulose	22000131	26778	40
Caelo	Hidroxietilcelulose	12249204	26782	40
Caelo	Hidroxietilcelulose	14352504	26790	60
Caelo	Hidroxietilcelulose	161006	26791	60
Caelo	Hidroxietilcelulose	16012909	26792	40
Caelo	Hidroxietilcelulose	16252003	26794	40
Caelo	Hidroxietilcelulose	16252008	26795	40
Caelo	Hidroxietilcelulose	16278705	26796	40
Caelo	Hidroxietilcelulose	173196	26798	40
Caelo	Hidroxietilcelulose	17115103	26799	40
Caelo	Hidroxietilcelulose	190769	26802	40
Caelo	Hidroxietilcelulose	190767	26803	40
Caelo	Hidroxietilcelulose	192602	26806	40
Caelo	Hidroxietilcelulose	21001636	26810	50
Caelo	Hidroxietilcelulose	20004006004	26811	40
Caelo	Hidroxietilcelulose	23001448	26854	40
Caelo	Hidroxietilcelulose	23002026	26966	40
Caelo	Hidroxietilcelulose	24001032	27220	40
Euro OTC	Hidroxietilcelulose	2211007	26780	40
Euro OTC	Hidroxietilcelulose	1110024-04	26783	40
Euro OTC	Hidroxietilcelulose	1606030	26786	40
Euro OTC	Hidroxietilcelulose	1610039	26787	40
Euro OTC	Hidroxietilcelulose	1711012	26800	40
Euro OTC	Hidroxietilcelulose	1804003	26801	40
Euro OTC	Hidroxietilcelulose	1907013	26804	40
Euro OTC	Hidroxietilcelulose	1911004	26805	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Hidroxietilcelulose	2008018	26807	40
Euro OTC	Hidroxietilcelulose	2101017	26808	40
Euro OTC	Hidroxietilcelulose	2302006	26814	40
Euro OTC	Hidroxietilcelulose	2305002	26815	40
Fagron	Hidroxietilcelulose	13H22-N11	26784	40
Fagron	Hidroxietilcelulose	16E09-B05-327042	26788	40
Fagron	Hidroxietilcelulose	20H03-B06-197061	26809	50
Fagron	Hidroxietilcelulose	21G14-B02-213646	26813	40
Fagron	Hidroxietilcelulose	23E11-B01-232178	26986	40
Caelo	Hidroxietilcelulose	22000131	26778SI	10
Caelo	Hidroxietilcelulose	16278705	26797	40
Caelo	Hidroxietilcelulose	20004006004	26811SI	10
Caelo	Hidroxietilcelulose	22000306	26812SI[†]	10
Euro OTC	Hidroxietilcelulose	2211007	26780SI	20
Euro OTC	Hidroxietilcelulose	2302006	26814SI	20
Fagron	Hidroxietilcelulose	21G14-B02-213646	26813SI	20

- 200 374 spectra from a total of 4006 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Hidroxietilcelulose*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hidroxietilcelulose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidroxietilcelulose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	1710	0	200 374
Type C	0	0	0	236 067

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Hidroxietilcelulose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6491 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26775	26775	0,00	136,25
26779	26779	0,00	161,13
26781	26781	0,00	150,86
26785	26785	0,00	170,24
26789	26781	49,90	176,03
26793	26793	0,00	148,13
26812	26812	0,00	190,85
26884	26884	0,00	174,03
27390	27390	0,00	184,27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hidroxitolueno butilado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21307-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hidroxitolueno butilado; BHT; Butilhidroxitolueno; Butylhydroxytoluenum

Special notes

When selecting the *Hidroxitolueno butilado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hidroxitolueno butilado	6	4	82

Second-stage model

For differentiation of the substance/substance group *Hidroxitolueno butilado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hidroxitolueno butilado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	103,01	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hidroxitolueno butilado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hidroxitolueno butilado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidroxitolueno butilado	13354602	21307	40	20131105
Caelo	Hidroxitolueno butilado	13354604	21355	40	AR-15-FG-007846-02
Caelo	Hidroxitolueno butilado	15172103	21911	60	20150529
Caelo	Hidroxitolueno butilado	15172103	22281	60	20150529
Caelo	Hidroxitolueno butilado	15172103	22350	60	20150529
Caelo	Hidroxitolueno butilado	190749	24554	40	20190405*
Caelo	Hidroxitolueno butilado	20000734	25552	40	20200324*
Caelo	Hidroxitolueno butilado	23000635	27322	40	20230503*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 380 spectra of 8 reference samples from the substance/substance group *Hidroxitolueno butilado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 582 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 7 reference samples from the substance/substance group *Hidroxitolueno butilado*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidroxitolueno butilado	163163	23356	40
Caelo	Hidroxitolueno butilado	180291	24019	40
Caelo	Hidroxitolueno butilado	21004127	25999	40
Caelo	Hidroxitolueno butilado	24002119	27440	40
Caelo	Hidroxitolueno butilado	21004127	25999SI	10
Caelo	Hidroxitolueno butilado	23000635	27322SI†	20
Caelo	Hidroxitolueno butilado	24002119	27440SI	20

- 201 874 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 834 spectra from 539 *Apo-Ident* customers from 85 batches from the substance/substance group *Hidroxitolueno butilado*.

- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Hidroxitolueno butilado	16316304	1
	Hidroxitolueno butilado	21004127001	2
	Hidroxitolueno butilado	22002085003	11
	Hidroxitolueno butilado	23000635001	7
	Hidroxitolueno butilado	23001370001	1
AHC	Hidroxitolueno butilado	23000635001	1
AHD	Hidroxitolueno butilado	18029102	1
Allianz Healthcare	Hidroxitolueno butilado	19074902	1
Apo Ident/ Noweda	Hidroxitolueno butilado	18029104	1
Bombastus	Hidroxitolueno butilado	13354604	1
Caelo	Hidroxitolueno butilado	11(18029107)	1
Caelo	Hidroxitolueno butilado	11131006	1
Caelo	Hidroxitolueno butilado	12(20000734001)	1
Caelo	Hidroxitolueno butilado	12158201	3
Caelo	Hidroxitolueno butilado	12158204	5
Caelo	Hidroxitolueno butilado	12207005	3
Caelo	Hidroxitolueno butilado	1220705	1
Caelo	Hidroxitolueno butilado	122080206	1
Caelo	Hidroxitolueno butilado	12280201	2
Caelo	Hidroxitolueno butilado	12280203	5
Caelo	Hidroxitolueno butilado	12280206	4
Caelo	Hidroxitolueno butilado	123823	1
Caelo	Hidroxitolueno butilado	12382302	5
Caelo	Hidroxitolueno butilado	12382304	7
Caelo	Hidroxitolueno butilado	12382307	1
Caelo	Hidroxitolueno butilado	12382309	8
Caelo	Hidroxitolueno butilado	12382312	1
Caelo	Hidroxitolueno butilado	13354602	4
Caelo	Hidroxitolueno butilado	13354604	8
Caelo	Hidroxitolueno butilado	13354609	2
Caelo	Hidroxitolueno butilado	13354611	4
Caelo	Hidroxitolueno butilado	1400501	1
Caelo	Hidroxitolueno butilado	1426801	1
Caelo	Hidroxitolueno butilado	143004502	1
Caelo	Hidroxitolueno butilado	14300501	11
Caelo	Hidroxitolueno butilado	14300502	8
Caelo	Hidroxitolueno butilado	14300503	2
Caelo	Hidroxitolueno butilado	14300505	6
Caelo	Hidroxitolueno butilado	14300506	2
Caelo	Hidroxitolueno butilado	15094501	12
Caelo	Hidroxitolueno butilado	15172101	11
Caelo	Hidroxitolueno butilado	15172103	21
Caelo	Hidroxitolueno butilado	15172105	12
Caelo	Hidroxitolueno butilado	15426801	13
Caelo	Hidroxitolueno butilado	1542680118029105	1
Caelo	Hidroxitolueno butilado	15426807	17
Caelo	Hidroxitolueno butilado	1631301	1
Caelo	Hidroxitolueno butilado	1631601	1
Caelo	Hidroxitolueno butilado	16316301	23
Caelo	Hidroxitolueno butilado	16316304	19
Caelo	Hidroxitolueno butilado	16316304-20180619Ma5	1
Caelo	Hidroxitolueno butilado	16316305	16
Caelo	Hidroxitolueno butilado	163163055402	1
Caelo	Hidroxitolueno butilado	16316307	29
Caelo	Hidroxitolueno butilado	18029102	22
Caelo	Hidroxitolueno butilado	18029104	8
Caelo	Hidroxitolueno butilado	18029105	44
Caelo	Hidroxitolueno butilado	18029107	24
Caelo	Hidroxitolueno butilado	18029108	13
Caelo	Hidroxitolueno butilado	1802915	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hidroxitolueno butilado	18048701	20
Caelo	Hidroxitolueno butilado	18229102	1
Caelo	Hidroxitolueno butilado	190749001	39
Caelo	Hidroxitolueno butilado	19074901	19
Caelo	Hidroxitolueno butilado	19074902	27
Caelo	Hidroxitolueno butilado	20000734001	26
Caelo	Hidroxitolueno butilado	2000734001	2
Caelo	Hidroxitolueno butilado	20161112-1	1
Caelo	Hidroxitolueno butilado	21000037001	40
Caelo	Hidroxitolueno butilado	21000037004	5
Caelo	Hidroxitolueno butilado	2100037001	1
Caelo	Hidroxitolueno butilado	21004127001	25
Caelo	Hidroxitolueno butilado	21004127002	9
Caelo	Hidroxitolueno butilado	2100427001	1
Caelo	Hidroxitolueno butilado	2113U02851	1
Caelo	Hidroxitolueno butilado	2170717	1
Caelo	Hidroxitolueno butilado	22002082001	1
Caelo	Hidroxitolueno butilado	22002085001	1
Caelo	Hidroxitolueno butilado	22002085003	4
Caelo	Hidroxitolueno butilado	220804(21004127001)	1
Caelo	Hidroxitolueno butilado	23000635001	1
Caelo	Hidroxitolueno butilado	231115BHT	1
Caelo	Hidroxitolueno butilado	2749	1
Caelo	Hidroxitolueno butilado	5426807	1
Caelo	Hidroxitolueno butilado	6316301	1
Caelo	Hidroxitolueno butilado	7031403	1
Caelo	Hidroxitolueno butilado	716M-02851	1
Caelo	Hidroxitolueno butilado	BT28112013	1
Caesar & Loretz /Gehe	Hidroxitolueno butilado	19074902	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	18029105	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21000037001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	190749001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	18029108	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	18029107	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21000037001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21000037004	1
Caesar & Loretz GmbH/AHD	Hidroxitolueno butilado	19074902	1
Caesar & Loretz GmbH/AHD	Hidroxitolueno butilado	21000037004	1
Caesar & Loretz GmbH/Gehe	Hidroxitolueno butilado	19074902	2
Caesar & Loretz GmbH/GEHE	Hidroxitolueno butilado	19074902	1
Caesar & Loretz GmbH/Gehe	Hidroxitolueno butilado	21000037001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	190749001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	19074902	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21004127001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21004127001	2
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21000037001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	18029107	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	19074902	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	20000734001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21000037001	1
Caesar & Loretz GmbH…	Hidroxitolueno butilado	21004127002	1
Caesar & Loretz GmbH	Hidroxitolueno butilado	18029102	1
Caesar & Loretz GmbH	Hidroxitolueno butilado	18029105	4
Caesar & Loretz GmbH	Hidroxitolueno butilado	18029107	3
Caesar & Loretz GmbH	Hidroxitolueno butilado	18029108	3
Caesar & Loretz GmbH	Hidroxitolueno butilado	190749001	10
Caesar & Loretz GmbH	Hidroxitolueno butilado	19074901	9
Caesar & Loretz GmbH	Hidroxitolueno butilado	19074902	8
Caesar & Loretz GmbH	Hidroxitolueno butilado	20000734001	15
Caesar & Loretz GmbH	Hidroxitolueno butilado	21000037001	12

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hidroxitolueno butilado	21000037004	6
Caesar & Loretz GmbH	Hidroxitolueno butilado	21004127001	12
Caesar & Loretz GmbH	Hidroxitolueno butilado	21004127002	7
Caesar & Loretz GmbH	Hidroxitolueno butilado	22002085001	1
Caesar & Loretz GmbH	Hidroxitolueno butilado	22002085003	3
Caesar & Loretz Hilden	Hidroxitolueno butilado	18029105	1
Caesar & Loretz/Noweda	Hidroxitolueno butilado	21000037001	1
Caesar & Loretz	Hidroxitolueno butilado	15426801	1
Caesar & Loretz	Hidroxitolueno butilado	16316307	1
Caesar Loretz	Hidroxitolueno butilado	190749001	1
Cealo / Otto Geilenk...	Hidroxitolueno butilado	18029108	1
Cealo/Sanacorp	Hidroxitolueno butilado	21004127001	1
Celo	Hidroxitolueno butilado	15426801	1
Euro OTC	Hidroxitolueno butilado	15172105	1
Euro OTC	Hidroxitolueno butilado	15426807	1
Euro OTC	Hidroxitolueno butilado	18029107	1
Fagron	Hidroxitolueno butilado	11308701	1
Fagron	Hidroxitolueno butilado	15426801	1
Fagron	Hidroxitolueno butilado	16316304	1
Fiebig	Hidroxitolueno butilado	15426807	1
Fiebig	Hidroxitolueno butilado	18029105	1
Gehe	Hidroxitolueno butilado	15426807	1
Gehe	Hidroxitolueno butilado	18029105	3
GEHE	Hidroxitolueno butilado	18029105	1
Gehe	Hidroxitolueno butilado	18029107	1
Gehe	Hidroxitolueno butilado	19074901	1
Gehe	Hidroxitolueno butilado	20000734001	2
Krieger	Hidroxitolueno butilado	16316301	1
Krieger	Hidroxitolueno butilado	18029108	1
L12	Hidroxitolueno butilado	15426807	1
L12	Hidroxitolueno butilado	16316307	1
Nachprüfung	Hidroxitolueno butilado	123456	1
Noweda	Hidroxitolueno butilado	12158201	1
Noweda	Hidroxitolueno butilado	12382304	1
Noweda	Hidroxitolueno butilado	15172103	1
Noweda	Hidroxitolueno butilado	15426807	1
Noweda	Hidroxitolueno butilado	16316305	1
Noweda	Hidroxitolueno butilado	18029105	2
Noweda	Hidroxitolueno butilado	21000037001	1
Noweda	Hidroxitolueno butilado	21004127002	1
Noweda	Hidroxitolueno butilado	23000635003	1
Phoenix	Hidroxitolueno butilado	12382305	1
Phoenix	Hidroxitolueno butilado	13354609	1
Phoenix	Hidroxitolueno butilado	15426801	1
Phoenix	Hidroxitolueno butilado	16316301	1
Phoenix	Hidroxitolueno butilado	20000734001	1
Phoenix	Hidroxitolueno butilado	21000037001	1
Phoenix	Hidroxitolueno butilado	22002085003	1
Phoenix	Hidroxitolueno butilado	3111201	1
Phönix/Caesar&Lorenz...	Hidroxitolueno butilado	22002085003	1
PHÖNIX	Hidroxitolueno butilado	16316304	1
Phönix	Hidroxitolueno butilado	16316307	1
Phönix	Hidroxitolueno butilado	18029102	1
Phönix	Hidroxitolueno butilado	190749001	1
Phönix	Hidroxitolueno butilado	19074901	1
PHÖNIX	Hidroxitolueno butilado	20000734001	1
Sanacorp	Hidroxitolueno butilado	13354609	1
Sanacorp	Hidroxitolueno butilado	14300505	1
sanacorp	Hidroxitolueno butilado	15172103	1
Sanacorp	Hidroxitolueno butilado	15172103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Hidroxitolueno butilado	16316305	1
Sanacorp	Hidroxitolueno butilado	18029105	1
Sanacorp	Hidroxitolueno butilado	2100037004	1
Sanacorp	Hidroxitolueno butilado	22002085003	1
Sanacorp	Hidroxitolueno butilado	23000635001	1
SanacorpWE:04.01.18 …	Hidroxitolueno butilado	16316304	1

- 235 233 spectra from 1515 *Apo-Ident* customers from a total of 49 176 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hidroxitolueno butilado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hidroxitolueno butilado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	210	0	201 874
Type C	0	829	5	235 233

The substance/substance group *Hidroxitolueno butilado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9007 %)	99.4005 % (> 99.0408 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21307	21355	7,82	236,32
21355	21355	0,00	241,73
21911	21355	9,17	240,81
22281	21355	6,03	245,70
22350	21355	7,06	241,16
24554	24554	0,00	254,17
25552	25552	0,00	244,97
27322	27322	0,00	251,43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Histidina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	23135-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Histidina; Histidinum

Special notes

When selecting the *Histidina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Histidina	6	4	1

Second-stage model

For differentiation of the substance/substance group *Histidina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Histidina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	115,89	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Histidina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Histidina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Histidina	1703022	23135	40	20170405*
Euro OTC	Histidina	2004038	25163	40	20200528*
Euro OTC	Histidina	2101009	25577	40	20210121*
Euro OTC	Histidina	2301009	26520	40	20230201*
Euro OTC	Histidina	2301009	26520SI	20	20230201*
Fagron	Histidina	15I01-B12-329082	23590	40	20150921
Fagron	Histidina	18J03-B02-355093	24701	40	20181123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Histidina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Histidina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Histidina	2201021	25953	40
Fagron	Histidina	17F15-B04-343276	23935	40
Fagron	Histidina	20J15-B01-202794	25487	40
Fagron	Histidina	23C07-B06-229457	26684	40
Euro OTC	Histidina	2201021	25953SI	10
Fagron	Histidina	23C07-B06-229457	26684SI	20

- 201 894 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Histidina*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Histidina	2004038-01	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Histidina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Histidina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	190	0	201 894
Type C	0	1	0	236 066

The substance/substance group *Histidina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23135	23135	0,00	186,79
23590	25577	5,53	187,73
24701	25577	4,86	187,79
25163	25163	0,00	186,70
25577	25577	0,00	186,89
26520	26520	0,00	188,12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ibuprofeno**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20205-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ibuprofeno; Ibuprofenum

Special notes

When selecting the *Ibuprofeno* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ibuprofeno	8	10	37

Second-stage model

For differentiation of the substance/substance group *Ibuprofeno* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ibuprofeno* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tretinoína	95,43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ibuprofeno* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ibuprofeno*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ibuprofeno	11352219	20774	40	20120124
Caelo	Ibuprofeno	172271	23641	40	20170831*
Caelo	Ibuprofeno	19000539	25190	40	20200316*
Caelo	Ibuprofeno	22003138	26484	40	20221020*
Euro OTC	Ibuprofeno	1211011-02	21248	40	1501533
Euro OTC	Ibuprofeno	1410025-02	23587	40	20141125
Euro OTC	Ibuprofeno	2004027	25278	40	20200603*
Euro OTC	Ibuprofeno	2208025	26339	40	20220915*
Euro OTC	Ibuprofeno	2208025	26339SI	20	20220915*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 340 spectra of 9 reference samples from the substance/substance group *Ibuprofeno*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 622 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 12 reference samples from the substance/substance group *Ibuprofeno*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ibuprofeno	13105108	21321	40
Caelo	Ibuprofeno	183003	24557	40
Caelo	Ibuprofeno	22002352	26359	40
Caelo	Ibuprofeno	22004099	26498	40
Caelo	Ibuprofeno	23000201	26722	40
Euro OTC	Ibuprofeno	2210019	26430	40
Euro OTC	Ibuprofeno	2301018	26521	40
Euro OTC	Ibuprofeno	2212017	26531	40
Euro OTC	Ibuprofeno	2301054	26575	40
Fagron	Ibuprofeno	23C20-B03-229831	26827	30
Caelo	Ibuprofeno	22002352	26359SI	20
Caelo	Ibuprofeno	22003138	26484SI†	20

- 201 654 spectra from a total of 4034 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 151 spectra from 76 *Apo-Ident* customers from 39 batches from the substance/substance group *Ibuprofeno*.
- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ibuprofeno	2210019-01	1
	Ibuprofeno	2212017-01	1
	Ibuprofeno	2301018-01	2
	Ibuprofeno	2301054-01	2
Audor Pharma	Ibuprofeno	2210019-01	5
Caelo	Ibuprofeno		1
Caelo	Ibuprofeno	1410025-02	1
Caelo	Ibuprofeno	17227101	1
Caelo	Ibuprofeno	17227102	1
Caelo	Ibuprofeno	17351401	3
Caelo	Ibuprofeno	17351403	1
Caelo	Ibuprofeno	17351410	1
Caelo	Ibuprofeno	183003002	1
Caelo	Ibuprofeno	18300303	1
Caelo	Ibuprofeno	18300304	2
Caelo	Ibuprofeno	21000655001	1
Caelo	Ibuprofeno	220002352001	1
Caelo	Ibuprofeno	22003138003	1
Caelo	Ibuprofeno	22003138004	1
Caelo	Ibuprofeno	22003138006	1
Caelo	Ibuprofeno	22004099001	1
Caelo	Ibuprofeno	2208025-01	1
Caelo	Ibuprofeno	2210019-01	1
Caesar & Loretz GmbH...	Ibuprofeno	18300304	1
Caesar & Loretz GmbH...	Ibuprofeno	183003002	1
Caesar & Loretz GmbH...	Ibuprofeno	21000655003	1
Caesar & Loretz GmbH	Ibuprofeno	183003002	1
Caesar & Loretz GmbH	Ibuprofeno	21000655001	4
Caesar & Loretz GmbH	Ibuprofeno	21000655004	1
Caesar & Loretz GmbH	Ibuprofeno	22002352001	2
Caesar & Loretz GmbH	Ibuprofeno	22003138004	2
Caesar & Loretz GmbH	Ibuprofeno	22004099001	4
Caesar & Loretz GmbH	Ibuprofeno	22004099003	1
Euro OTC	Ibuprofeno	1211011-01	1
Euro OTC	Ibuprofeno	1410025-01	6
Euro OTC	Ibuprofeno	1410025-02	7
Euro OTC	Ibuprofeno	2004027-01	2
Euro OTC	Ibuprofeno	2004027-02	2
Euro OTC	Ibuprofeno	2208025	1
Euro OTC	Ibuprofeno	220802501	1
Euro OTC	Ibuprofeno	2208025-01	30
Euro OTC	Ibuprofeno	220825-01	1
Euro OTC	Ibuprofeno	2210019-01	22
Euro OTC	Ibuprofeno	2210019-02	7
Euro OTC	Ibuprofeno	221201701	1
Euro OTC	Ibuprofeno	2212017-01	1
Euro OTC	Ibuprofeno	2301018-01	5
Euro OTC	Ibuprofeno	7050-4896	2
Euro OTC	Ibuprofeno	9061807	1
Euro/Sanacorp	Ibuprofeno	2208025-01	2
Fagron	Ibuprofeno	22K07-B12-224949	2
GEHE	Ibuprofeno	15103011	1
GEHE	Ibuprofeno	22003138004	1
Gehe	Ibuprofeno	22003138008	3
Jenne	Ibuprofeno	22003138003	2

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 916 spectra from 1515 *Apo-Ident* customers from a total of 49 219 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ibuprofeno* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ibuprofeno* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	430	0	201 654
Type C	0	151	0	235 916

The substance/substance group *Ibuprofeno* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.0265 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20774	26339	12,47	97,97
21248	21248	0,00	99,35
23587	25278	6,46	98,87
23641	23641	0,00	99,82
25190	25190	0,00	97,14
25278	25278	0,00	99,42
26339	26339	0,00	95,43
26484	26484	0,00	95,63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Indometacina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20720-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Indometacina; Indometacinum

Special notes

When selecting the *Indometacina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Indometacina	6	4	33

Second-stage model

For differentiation of the substance/substance group *Indometacina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Indometacina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	114,41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Indometacina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Indometacina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Indometacina	1012009-02	20720	40	1402050
Euro OTC	Indometacina	1205002-01	21327	40	20120521
Euro OTC	Indometacina	1512031	22291	60	20160122*
Euro OTC	Indometacina	1612017	22981	40	20170209*
Fagron	Indometacina	18H14-B04-365453	25062	40	20180920
Fagron	Indometacina	21E12-F04-379312	25841	50	20210811

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 6 reference samples from the substance/substance group *Indometacina*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 692 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Indometacina*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Indometacina	1801040	23969	40
Euro OTC	Indometacina	2106012	25762	40
Fagron	Indometacina	17I08-B06-339738	23715	40
Fagron	Indometacina	23C04-B10-230386	26896	30
Fagron	Indometacina	21E12-F04-379312	25841SI†	10
Fagron	Indometacina	23C04-B10-230386	26896SI	20

- 201 904 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 153 spectra from 75 *Apo-Ident* customers from 35 batches from the substance/substance group *Indometacina*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Indometacina	2106012-01	1
	Indometacina	2106012-02	3
apo-ident	Indometacina	1801040-01	1
Caelo	Indometacina	1512031-01	1
Caelo	Indometacina	1801040-01	3
Caelo	Indometacina	1801040-02	1
Euro OTC	Indometacina	1202002-02	1
Euro OTC	Indometacina	1205002-01	2
Euro OTC	Indometacina	1205002-02	2
Euro OTC	Indometacina	1512031-01	17
Euro OTC	Indometacina	16110102	1
Euro OTC	Indometacina	161201-02	1
Euro OTC	Indometacina	1612017-01	9
Euro OTC	Indometacina	1612017-02	9
Euro OTC	Indometacina	1612017-2	1
Euro OTC	Indometacina	180104001	2
Euro OTC	Indometacina	1801040-01	25
Euro OTC	Indometacina	180104002	1
Euro OTC	Indometacina	1801040-02	19
Euro OTC	Indometacina	1801040-03	5
Euro OTC	Indometacina	1801044-02	1
Euro OTC	Indometacina	201606272030	1
Euro OTC	Indometacina	201612162018	2
Euro OTC	Indometacina	2091716	1
Euro OTC	Indometacina	2100012-01	1
Euro OTC	Indometacina	2106012-01	16
Euro OTC	Indometacina	2106012-12	1
Euro OTC	Indometacina	27101709	1
Euro OTC	Indometacina	612017-02	1
Euro/ Euro	Indometacina	1801040-01	1
Euro/Krieger	Indometacina	1801040-02	1
Fagron	Indometacina		1
Fagron	Indometacina	14I08-B06-343286	1
Fagron	Indometacina	14I25-B02-303648	1
Fagron	Indometacina	15L09-B08-315982	1
Fagron	Indometacina	17I08B06	1
Fagron	Indometacina	17I08-B06-339738	2
Fagron	Indometacina	17I08-B06-343286	1
Fagron	Indometacina	18H14-B03-352947	1
Fagron	Indometacina	18H14-B03-359139	1
Fagron	Indometacina	18H14-B04-368823	1
Gehe	Indometacina	1512031-01	1
Krieger/Euro	Indometacina	4932195	1
Noweda	Indometacina	1801040-01	3
Sanacorp	Indometacina	1612017-02	1
Sanacorp	Indometacina	1801040-03	1
Sanacorp	Indometacina	2106012-01	2
Sanacorp	Indometacina	2106012-02	1

- 235 914 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Indometacina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

relevant spectra of the various substances were compared with *Indometacina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	180	0	201 904
Type C	0	152	1	235 914

The substance/substance group *Indometacina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	99.3464 % (> 97.3856 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20720	20720	0,00	193,93
21327	20720	7,00	194,71
22291	22291	0,00	192,66
22981	22981	0,00	194,35
25062	22291	6,00	195,93
25841	22981	6,81	200,16

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Iodofórmio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20094-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Iodofórmio; Iodoformium

Special notes

When selecting the *Iodofórmio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Iodofórmio	7	8	166

Second-stage model

For differentiation of the substance/substance group *Iodofórmio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Iodofórmio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	197,45	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Iodofórmio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Iodofórmio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Iodofórmio	12283206	21297	40	20130709
Caelo	Iodofórmio	16012302	23192	40	AR-17-FG-012459-01
Caelo	Iodofórmio	16012302	23407	40	20160211
Caelo	Iodofórmio	191132	24710	40	20190524*
Caelo	Iodofórmio	21000186	25647	40	20210316*
Caelo	Iodofórmio	21000181	25648	40	20210330*
Caelo	Iodofórmio	22003551	26627	40	20230130*
Fagron	Iodofórmio	12L11-B41	21278	40	20140113

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Iodofórmio*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 350 spectra of 11 reference samples from the substance/substance group *Iodofórmio*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Iodofórmio	170860	23652	30
Caelo	Iodofórmio	180919	24012	40
Caelo	Iodofórmio	182495	24380	40
Caelo	Iodofórmio	22000203	26020	40
Caelo	Iodofórmio	22000204	26021	40
Caelo	Iodofórmio	22003550	26628	40
Caelo	Iodofórmio	24000893	27238	40
Caelo	Iodofórmio	24000892	27263	40
Caelo	Iodofórmio	22000203	26020SI	10
Caelo	Iodofórmio	22000204	26021SI	10
Caelo	Iodofórmio	22003551	26627SI†	20

- 201 734 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 783 spectra from 302 *Apo-Ident* customers from 169 batches from the substance/substance group *Iodofórmio*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 166 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Iodofórmio	22000203005	1
	Iodofórmio	22000203006	3
	Iodofórmio	22000204001	2
	Iodofórmio	22003550002	1
	Iodofórmio	22003550003	1
	Iodofórmio	22003551002	1
	Iodofórmio	22003551003	1
	Iodofórmio	22003607002	2
	Iodofórmio	22003607003	1
AHC	Iodofórmio	22003550003	1
AHC	Iodofórmio	22003551002	1
AHC	Iodofórmio	22003551005	1
AHD	Iodofórmio	22000204001	2
AHD	Iodofórmio	22003551002	2
AHD	Iodofórmio	22003607002	1
cae	Iodofórmio	191132003	1
Caelo	Iodofórmio	1010316	1
Caelo	Iodofórmio	10320407	1
Caelo	Iodofórmio	12070102	2
Caelo	Iodofórmio	12070105	1
Caelo	Iodofórmio	12070303	2
Caelo	Iodofórmio	12070407	1
Caelo	Iodofórmio	12070501	1
Caelo	Iodofórmio	12070502	1
Caelo	Iodofórmio	12070601	4
Caelo	Iodofórmio	12070602	3
Caelo	Iodofórmio	12070605	1
Caelo	Iodofórmio	12070606	2
Caelo	Iodofórmio	12070608	3
Caelo	Iodofórmio	12150902	6
Caelo	Iodofórmio	12150903	1
Caelo	Iodofórmio	12150905	3
Caelo	Iodofórmio	12150907	1
Caelo	Iodofórmio	12150908	4
Caelo	Iodofórmio	12150910	6
Caelo	Iodofórmio	12283201	3
Caelo	Iodofórmio	12283202	5
Caelo	Iodofórmio	12283206	3
Caelo	Iodofórmio	12283303	2
Caelo	Iodofórmio	12283304	1
Caelo	Iodofórmio	12283307	1
Caelo	Iodofórmio	14077601	1
Caelo	Iodofórmio	14077602	1
Caelo	Iodofórmio	14077603	2
Caelo	Iodofórmio	14077606	2
Caelo	Iodofórmio	14077607	1
Caelo	Iodofórmio	14077702	7
Caelo	Iodofórmio	14229504	2
Caelo	Iodofórmio	14229505	1
Caelo	Iodofórmio	14229507	3
Caelo	Iodofórmio	14229508	2
Caelo	Iodofórmio	14230001	6
Caelo	Iodofórmio	14230002	3
Caelo	Iodofórmio	14230003	1
Caelo	Iodofórmio	14230006	5
Caelo	Iodofórmio	14230007	3
Caelo	Iodofórmio	14230008	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Iodofórmio	14230302	2
Caelo	Iodofórmio	14230304	2
Caelo	Iodofórmio	14230305	9
Caelo	Iodofórmio	14230306	6
Caelo	Iodofórmio	14230308	6
Caelo	Iodofórmio	1527104	1
Caelo	Iodofórmio	15276001	3
Caelo	Iodofórmio	15276002	6
Caelo	Iodofórmio	15276101	6
Caelo	Iodofórmio	15276102	5
Caelo	Iodofórmio	15276103	5
Caelo	Iodofórmio	15276104	4
Caelo	Iodofórmio	15276105	8
Caelo	Iodofórmio	15276107	1
Caelo	Iodofórmio	15276108	3
Caelo	Iodofórmio	15276109	3
Caelo	Iodofórmio	1527611	1
Caelo	Iodofórmio	15276111	6
Caelo	Iodofórmio	15276113	1
Caelo	Iodofórmio	1576103	1
Caelo	Iodofórmio	16012201	10
Caelo	Iodofórmio	16012202	2
Caelo	Iodofórmio	16012204	6
Caelo	Iodofórmio	16012205	2
Caelo	Iodofórmio	16012206	6
Caelo	Iodofórmio	16012207	7
Caelo	Iodofórmio	16012210	6
Caelo	Iodofórmio	16012302	5
Caelo	Iodofórmio	16012305	6
Caelo	Iodofórmio	16012306	8
Caelo	Iodofórmio	16012308	3
Caelo	Iodofórmio	16012309	5
Caelo	Iodofórmio	16012311	1
Caelo	Iodofórmio	17086001	6
Caelo	Iodofórmio	17086002	4
Caelo	Iodofórmio	17086003	5
Caelo	Iodofórmio	17086004	10
Caelo	Iodofórmio	17086005	10
Caelo	Iodofórmio	17086006	12
Caelo	Iodofórmio	17086008	3
Caelo	Iodofórmio	17086012	3
Caelo	Iodofórmio	17086066	1
Caelo	Iodofórmio	18041821	1
Caelo	Iodofórmio	18091801	1
Caelo	Iodofórmio	18091802	7
Caelo	Iodofórmio	18091803	1
Caelo	Iodofórmio	18091804	4
Caelo	Iodofórmio	18091805	17
Caelo	Iodofórmio	18091806	10
Caelo	Iodofórmio	18091807	2
Caelo	Iodofórmio	18091902	1
Caelo	Iodofórmio	18091904	1
Caelo	Iodofórmio	18091905	16
Caelo	Iodofórmio	18091906	4
Caelo	Iodofórmio	18091907	2
Caelo	Iodofórmio	18091909	4
Caelo	Iodofórmio	18091911	4
Caelo	Iodofórmio	18091912	6
Caelo	Iodofórmio	18091912P-200326-10	1
Caelo	Iodofórmio	18249501	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Iodofórmio	18249502	11
Caelo	Iodofórmio	18249503	6
Caelo	Iodofórmio	1911320004	1
Caelo	Iodofórmio	191132001	13
Caelo	Iodofórmio	191132002	9
Caelo	Iodofórmio	191132004	19
Caelo	Iodofórmio	191132005	6
Caelo	Iodofórmio	19113201	14
Caelo	Iodofórmio	19113204	2
Caelo	Iodofórmio	1961132001	1
Caelo	Iodofórmio	1961132004	1
Caelo	Iodofórmio	20000241001	17
Caelo	Iodofórmio	20000241004	4
Caelo	Iodofórmio	20000241005	5
Caelo	Iodofórmio	20000241006	12
Caelo	Iodofórmio	20000241007	1
Caelo	Iodofórmio	20000241008	12
Caelo	Iodofórmio	20000241009	1
Caelo	Iodofórmio	21000181003	7
Caelo	Iodofórmio	21000181004	3
Caelo	Iodofórmio	21000186001	9
Caelo	Iodofórmio	21000186002	15
Caelo	Iodofórmio	21000186003	3
Caelo	Iodofórmio	21000186006	8
Caelo	Iodofórmio	21000186007	1
Caelo	Iodofórmio	21000186009	1
Caelo	Iodofórmio	21000191003	1
Caelo	Iodofórmio	2100186006	1
Caelo	Iodofórmio	21051305	1
Caelo	Iodofórmio	22000203001	3
Caelo	Iodofórmio	22000203006	1
Caelo	Iodofórmio	22000204001	1
Caelo	Iodofórmio	22000204002	2
Caelo	Iodofórmio	22000204004	1
Caelo	Iodofórmio	22003607002	4
Caelo	Iodofórmio	22003607003	1
Caelo	Iodofórmio	220127	1
Caelo	Iodofórmio	23021715	1
Caelo	Iodofórmio	28011503	1
Caelo	Iodofórmio	3041407	1
Caelo	Iodofórmio	320E01726	1
Caelo	Iodofórmio	46(18091805)	1
Caelo	Iodofórmio	47(18091905)	1
Caelo	Iodofórmio	48(18091905)	1
Caelo	Iodofórmio	49(18091911)	1
Caelo	Iodofórmio	52(20000241001)	1
Caelo	Iodofórmio	53(20000241001)	1
Caelo	Iodofórmio	54(20000241008)	2
Caelo	Iodofórmio	55(20000241001)	1
Caeolo/Sanacorp	Iodofórmio	21000181003	1
Caesar & Loretz GmbH...	Iodofórmio	21000181003	4
Caesar & Loretz GmbH...	Iodofórmio	18091906	1
Caesar & Loretz GmbH...	Iodofórmio	18249502	1
Caesar & Loretz GmbH...	Iodofórmio	12070501	3
Caesar & Loretz GmbH...	Iodofórmio	191132001	2
Caesar & Loretz GmbH...	Iodofórmio	19113201	1
Caesar & Loretz GmbH...	Iodofórmio	21000186001	1
Caesar & Loretz GmbH...	Iodofórmio	191132001	1
Caesar & Loretz GmbH/Gehe	Iodofórmio	21000186001	1
Caesar & Loretz GmbH/GEHE	Iodofórmio	21000186001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Iodofórmio	191132001	4
Caesar & Loretz GmbH...	Iodofórmio	191132004	1
Caesar & Loretz GmbH...	Iodofórmio	21000186003	1
Caesar & Loretz GmbH...	Iodofórmio	AP220630-03	1
Caesar & Loretz GmbH...	Iodofórmio	AP221112-01	1
Caesar & Loretz GmbH...	Iodofórmio	21000186003	1
Caesar & Loretz GmbH...	Iodofórmio	18249502	1
Caesar & Loretz GmbH...	Iodofórmio	191132001	1
Caesar & Loretz GmbH...	Iodofórmio	19113203	1
Caesar & Loretz GmbH...	Iodofórmio	19113204	1
Caesar & Loretz GmbH...	Iodofórmio	20000241002	2
Caesar & Loretz GmbH...	Iodofórmio	20000241004	1
Caesar & Loretz GmbH...	Iodofórmio	AP220812-01	2
Caesar & Loretz GmbH	Iodofórmio	12150907	1
Caesar & Loretz GmbH	Iodofórmio	18091902	2
Caesar & Loretz GmbH	Iodofórmio	18091905	4
Caesar & Loretz GmbH	Iodofórmio	18091906	1
Caesar & Loretz GmbH	Iodofórmio	18091909	1
Caesar & Loretz GmbH	Iodofórmio	18091911	1
Caesar & Loretz GmbH	Iodofórmio	18091912	1
Caesar & Loretz GmbH	Iodofórmio	18249502	8
Caesar & Loretz GmbH	Iodofórmio	191132001	6
Caesar & Loretz GmbH	Iodofórmio	191132002	1
Caesar & Loretz GmbH	Iodofórmio	191132004	3
Caesar & Loretz GmbH	Iodofórmio	191132005	2
Caesar & Loretz GmbH	Iodofórmio	19113201	6
Caesar & Loretz GmbH	Iodofórmio	19113203	1
Caesar & Loretz GmbH	Iodofórmio	19113204	1
Caesar & Loretz GmbH	Iodofórmio	20000241001	4
Caesar & Loretz GmbH	Iodofórmio	20000241005	3
Caesar & Loretz GmbH	Iodofórmio	20000241006	2
Caesar & Loretz GmbH	Iodofórmio	20000241008	5
Caesar & Loretz GmbH	Iodofórmio	20000241009	1
Caesar & Loretz GmbH	Iodofórmio	21000181003	4
Caesar & Loretz GmbH	Iodofórmio	21000186001	1
Caesar & Loretz GmbH	Iodofórmio	21000186002	5
Caesar & Loretz GmbH	Iodofórmio	21000186003	4
Caesar & Loretz GmbH	Iodofórmio	21000186004	1
Caesar & Loretz GmbH	Iodofórmio	21000186006	1
Caesar & Loretz GmbH	Iodofórmio	21000186007	2
Caesar & Loretz GmbH	Iodofórmio	22000203001	1
Caesar & Loretz GmbH	Iodofórmio	22000204002	1
Caesar & Loretz GmbH	Iodofórmio	22003607002	1
Caesar & Loretz GmbHGehe	Iodofórmio	18249502	1
Caesar & Loretz Hilden	Iodofórmio	18091905	2
Caesar Loretz	Iodofórmio	20000241001	1
Caesar u.Loretz	Iodofórmio	16012209	2
Cao	Iodofórmio	18249503	1
Cesar&Loretz GmbH Noweda	Iodofórmio	19113201	1
Euro OTC	Iodofórmio	14229504	2
Fagron	Iodofórmio	12E30-N01	2
Fagron	Iodofórmio	12L11-B41	1
Fagron	Iodofórmio	12L11-B41-290055	1
Fagron	Iodofórmio	14229508	1
Fagron	Iodofórmio	14D09-B14-293029	1
Fagron	Iodofórmio	16012302	1
Fagron	Iodofórmio	18091803	1
Fiebig	Iodofórmio	16012206	1
fragon	Iodofórmio	12283303	1
Gehe	Iodofórmio	14230008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Iodofórmio	17086001	1
GEHE	Iodofórmio	17086002	1
GEHE	Iodofórmio	17086003	1
Gehe	Iodofórmio	191132001	1
Gehe	Iodofórmio	22003551003	1
Henry Lamotte Oils G…	Iodofórmio	16012309	1
Kehr	Iodofórmio	22003607003	1
Midas	Iodofórmio	16012306	1
Nachprüfung von Juni 2018	Iodofórmio	15276103	1
Noweda /Cealo	Iodofórmio	20000241005	1
Noweda	Iodofórmio	10320402	1
Noweda	Iodofórmio	12070407	1
Noweda	Iodofórmio	17086012	1
Noweda	Iodofórmio	18091805	1
Noweda	Iodofórmio	18091806	1
Noweda	Iodofórmio	18091902	1
Noweda	Iodofórmio	19113201	1
Noweda	Iodofórmio	20000241008	2
Noweda	Iodofórmio	21000186002	1
Noweda	Iodofórmio	22000204001	1
Phoenix	Iodofórmio	12070601	1
Phoenix	Iodofórmio	191132001	1
Phoenix	Iodofórmio	22003607003	1
phönix	Iodofórmio	18249502	2
Sanacorp	Iodofórmio	17086005	1
Sanacorp	Iodofórmio	18091805	1
Sanacorp	Iodofórmio	22003551002	1
Sanacorp	Iodofórmio	22003607003	2

- 235 284 spectra from 1515 *Apo-Ident* customers from a total of 49 091 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Iodofórmio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Iodofórmio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	350	0	201 734
Type C	0	777	6	235 284

The substance/substance group *Iodofórmio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9007 %)	99.2337 % (> 98.8506 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21278	23192	20,90	233,61
21297	26627	28,89	228,92
23192	23192	0,00	241,72
23407	23192	13,59	239,05
24710	24710	0,00	243,64
25647	25647	0,00	243,85
25648	25648	0,00	242,29
26627	26627	0,00	233,22

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Iodopovidona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20472-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Iodopovidona; Povidonum iodinatum

Special notes

When selecting the *Iodopovidona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Iodopovidona	17	6	57

Second-stage model

For differentiation of the substance/substance group *Iodopovidona* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Iodopovidona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Povidona	21,14	16,46
Ácido fusídico	61,49	46,41
⋮	⋮	⋮
Progesterona	85,15	52,91
Espironolactona	>50	53,79
Propionato de testosterona	>50	78,19
Ubidecarenona	>50	137,77

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Iodopovidona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Iodopovidona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Iodopovidona	13337205	21466	60	20131021
Caelo	Iodopovidona	15234101	23252	40	AR-17-FG-015433-02
Caelo	Iodopovidona	15234109	23256	40	20150717
Caelo	Iodopovidona	182385	24234	40	20180917*
Caelo	Iodopovidona	20003244	25659	40	20210106*
Caelo	Iodopovidona	22001868	26238	40	20220720*
Caelo	Iodopovidona	23000265	26725	40	20230331*
Euro OTC	Iodopovidona	1501029-01	21777	60	20150211
Euro OTC	Iodopovidona	1509009	21908	60	20150918*
Euro OTC	Iodopovidona	1606026-02	23906	40	20160708
Euro OTC	Iodopovidona	1805007	24118	40	20180525*
Euro OTC	Iodopovidona	1905008	24770	40	20190628*
Euro OTC	Iodopovidona	2001048	25122	40	20200320*
Euro OTC	Iodopovidona	2003030	25240	40	20200707*
Euro OTC	Iodopovidona	2009042	25433	40	20201022*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Iodopovidona	2206025	26225	40	20220721*
Euro OTC	Iodopovidona	2206025	26225SI	20	20220721*
Euro OTC	Iodopovidona	2305022	26750	40	20230705*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 760 spectra of 18 reference samples from the substance/substance group *Iodopovidona*. These samples are listed above in the *calibration samples* section. The reference samples come from 17 different batches.
- 152 202 spectra from a total of 2825 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Iodopovidona*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Iodopovidona	180763	24261	40
Caelo	Iodopovidona	192297	24879	40
Euro OTC	Iodopovidona	1606026	22675	40
Euro OTC	Iodopovidona	1704007	23435	40
Euro OTC	Iodopovidona	2202017	26044	40
Euro OTC	Iodopovidona	2406008	27295	40
Caelo	Iodopovidona	22001868	26238SI†	20
Euro OTC	Iodopovidona	2202017	26044SI	10

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 814 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 199 spectra from 75 *Apo-Ident* customers from 63 batches from the substance/substance group *Iodopovidona*.
- Among them are spectra of independent samples from 57 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Iodopovidona	22001868001	2
	Iodopovidona	22001868004	2
	Iodopovidona	2206025	1
	Iodopovidona	2206025-01	2
apo ident	Iodopovidona	1606026-02	4
apo-ident	Iodopovidona	1606026-02	1
Audor Pharma	Iodopovidona	2009042-01	1
BASF, Noweda	Iodopovidona	1110013-02	1
Basf/Sanacorp	Iodopovidona	180500701	1
Basf/Sanacorp	Iodopovidona	2009042-01	1
Caelo	Iodopovidona	1110013-02	1
Caelo	Iodopovidona	11168607	1
Caelo	Iodopovidona	11168612	1
Caelo	Iodopovidona	12072605	1
Caelo	Iodopovidona	12153106	2
Caelo	Iodopovidona	12153110	2
Caelo	Iodopovidona	12153116	2
Caelo	Iodopovidona	12153119	2
Caelo	Iodopovidona	1407032-01	1
Caelo	Iodopovidona	14195810	2
Caelo	Iodopovidona	15121402	1
Caelo	Iodopovidona	15234101	1
Caelo	Iodopovidona	15234109	1
Caelo	Iodopovidona	15442405	1
Caelo	Iodopovidona	17028102	2
Caelo	Iodopovidona	18025301	1
Caelo	Iodopovidona	1805007-01	1
Caelo	Iodopovidona	18076308	1
Caelo	Iodopovidona	1905008-01	1
Caelo	Iodopovidona	19061302	1
Caelo	Iodopovidona	192297004	6
Caelo	Iodopovidona	20003244001	4
Caelo	Iodopovidona	20003244004	2
Caelo	Iodopovidona	21001575002	2
Caelo	Iodopovidona	21001575004	1
Caelo	Iodopovidona	22001868004	1
Caesar & Loretz GmbH...	Iodopovidona	19075002	1
Caesar & Loretz GmbH	Iodopovidona	18076308	1
Caesar & Loretz GmbH	Iodopovidona	19075003	1
Caesar & Loretz GmbH	Iodopovidona	192297002	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Iodopovidona	192297003	1
Caesar & Loretz GmbH	Iodopovidona	20003244001	4
Caesar & Loretz GmbH	Iodopovidona	20003244006	1
Caesar & Loretz GmbH	Iodopovidona	20004050001	1
Caesar & Loretz GmbH	Iodopovidona	2003244001	1
Caesar & Loretz GmbH	Iodopovidona	21001575002	1
EuRho/Noweda	Iodopovidona	2009042-02	1
EuRho	Iodopovidona	2003030-01	2
Euro OTC	Iodopovidona	110013-02	1
Euro OTC	Iodopovidona	111001302	1
Euro OTC	Iodopovidona	1110013-02	4
Euro OTC	Iodopovidona	130901001	1
Euro OTC	Iodopovidona	1401029-01	1
Euro OTC	Iodopovidona	1407032-01	5
Euro OTC	Iodopovidona	1509009-01	2
Euro OTC	Iodopovidona	1509009-02	2
Euro OTC	Iodopovidona	1603023-01	2
Euro OTC	Iodopovidona	1606026	1
Euro OTC	Iodopovidona	1606026-02	13
Euro OTC	Iodopovidona	1704007-01	2
Euro OTC	Iodopovidona	1704007-02	2
Euro OTC	Iodopovidona	180500701	1
Euro OTC	Iodopovidona	1805007-01	7
Euro OTC	Iodopovidona	1805007-02	8
Euro OTC	Iodopovidona	1905008	1
Euro OTC	Iodopovidona	190500801	1
Euro OTC	Iodopovidona	1905008-01	26
Euro OTC	Iodopovidona	2001048-01	1
Euro OTC	Iodopovidona	2003030-01	10
Euro OTC	Iodopovidona	2009042-01	7
Euro OTC	Iodopovidona	2009042-02	5
Euro OTC	Iodopovidona	2202017-01	1
Euro OTC	Iodopovidona	2206025-01	1
Euro OTC	Iodopovidona	8051808	1
Euro OTC	Iodopovidona	G4208BPZ0	2
Euro/ Jenne	Iodopovidona	1606026-02	4
Euroo/Phoenix	Iodopovidona	G3115BPZ0	1
Euroo/Sana	Iodopovidona	1501029-01	3
Fagron	Iodopovidona	1110013-02	1
Noweda	Iodopovidona	G0354BPZ0	1
ph euro	Iodopovidona	19050080-01	1
Phoenix	Iodopovidona	2003030-01	1
Phönix	Iodopovidona	1110013-02	1
Sanacorp	Iodopovidona	2202017-01	1
Sanacorp	Iodopovidona	2406008-01	1
Stumpf	Iodopovidona	11168612	1

- 235 868 spectra from 1515 *Apo-Ident* customers from a total of 49 196 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Iodopovidona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Iodopovidona* and it was evaluated

how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	760	0	152 202
Type B	0	265	5	201 814
Type C	0	188	11	235 868

The substance/substance group *Iodopovidona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2105 %)
Type B	100.0000 % (> 99.9912 %)	98.1481 % (> 97.0370 %)
Type C	100.0000 % (> 99.9007 %)	94.4724 % (> 92.9648 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21466	21908	7,66	49,97
21777	21908	6,48	52,17
21908	21908	0,00	59,71
23252	23252	0,00	56,99
23256	23252	15,08	53,49
23906	21908	11,67	47,15
24118	24118	0,00	159,21
24234	24234	0,00	50,05
24770	24770	0,00	52,72
25122	25122	0,00	47,04
25240	25240	0,00	49,49
25433	25433	0,00	49,62
25659	25659	0,00	48,24
26225	26225	0,00	55,76
26238	26238	0,00	151,69
26725	26725	0,00	135,50
26750	26750	0,00	26,56

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Isoleucina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21045-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Isoleucina; Isoleucinum

Special notes

When selecting the *Isoleucina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Isoleucina	7	14	16

Second-stage model

For differentiation of the substance/substance group *Isoleucina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Isoleucina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Leucina	62,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Isoleucina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Isoleucina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Isoleucina	1604057	22566	40	20160601*
Euro OTC	Isoleucina	1704022	23386	40	20170612*
Euro OTC	Isoleucina	1909025	24931	40	20191015*
Euro OTC	Isoleucina	2301011	26534	40	20230201*
Euro OTC	Isoleucina	2301011	26534SI	20	20230201*
Fagron	Isoleucina	13E02-B01-286930	21045	40	1403154
Fagron	Isoleucina	13E02-B01	21332	40	20130621
Fagron	Isoleucina	20B12-B01-197402	25441	40	20200313

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 8 reference samples from the substance/substance group *Isoleucina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 17 reference samples from the substance/substance group *Isoleucina*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Isoleucina	1611007	22869	40
Euro OTC	Isoleucina	1708027	23702	40
Euro OTC	Isoleucina	1711034	23869	40
Euro OTC	Isoleucina	1803019	24080	40
Euro OTC	Isoleucina	1805013	24115	40
Euro OTC	Isoleucina	1901010	24515	40
Euro OTC	Isoleucina	2101041	25530	40
Euro OTC	Isoleucina	2111017	25891	50
Euro OTC	Isoleucina	2309020	27011	40
Euro OTC	Isoleucina	2404003	27288	40
Fagron	Isoleucina	21B01-B06-210568	26292	40
Fagron	Isoleucina	22G01-B04-221842	26682	40
Fagron	Isoleucina	23C07-B07-230992	27043	40
Fagron	Isoleucina	24A10-B08-235292	27425	40
Euro OTC	Isoleucina	2111017	25891SI	10
Fagron	Isoleucina	21B01-B06-210568	26292SI	20
Fagron	Isoleucina	22G01-B04-221842	26682SI	20

- 201 464 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 12 *Apo-Ident* customers from 17 batches from the substance/substance group *Isoleucina*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Isoleucina	1704022-01	1
Euro OTC	Isoleucina	1708027-01	1
Euro OTC	Isoleucina	1711034-01	1
Euro OTC	Isoleucina	1805013-02	1
Euro OTC	Isoleucina	1901010-01	1
Euro OTC	Isoleucina	2006027-01	5
Euro OTC	Isoleucina	2101041-01	1
Euro OTC	Isoleucina	2111017-01	5
Fagro WE:19.05.16 EK...	Isoleucina	15A14-B09-314881	1
Fagron	Isoleucina	12080167	1
Fagron	Isoleucina	13A22-N03	1
Fagron	Isoleucina	13E02-B01-286930	1
Fagron	Isoleucina	14D08-B02-296089	2
Fagron	Isoleucina	16H24-B03-331739	1
Fagron	Isoleucina	17010483	2
Fagron	Isoleucina	17H14-B04-339008	5
Sanacorp	Isoleucina	17H14-B04-339008	1
Synop WE:18.12.17 E...	Isoleucina	17H14-B04-339009	1

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Isoleucina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Isoleucina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	620	0	201 464
Type C	0	32	0	236 035

The substance/substance group *Isoleucina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.2500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21045	21045	0,00	102,70
21332	21045	4,84	102,24
22566	22566	0,00	106,57
23386	23386	0,00	107,27
24931	24931	0,00	105,05
25441	26534	5,12	109,58
26534	26534	0,00	106,23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lactato de cálcio penta-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20745-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lactato de cálcio penta-hidratado; Calcii lactas pentahydricus

Special notes

When selecting the *Lactato de cálcio penta-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lactato de cálcio penta-hidratado	7	5	46

Second-stage model

For differentiation of the substance/substance group *Lactato de cálcio penta-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lactato de cálcio penta-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	48,93	–
Fosfato sódico de riboflavina hidratado	53,06	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lactato de cálcio penta-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lactato de cálcio penta-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lactato de cálcio penta-h…	15101401	21909	60	20150407
Caelo	Lactato de cálcio penta-h…	15101405	22263	60	20150407
Caelo	Lactato de cálcio penta-h…	161313	22445	60	20160513*
Caelo	Lactato de cálcio penta-h…	20000512	25225	40	20200320*
Caelo	Lactato de cálcio penta-h…	23002025	26971	40	20230918*
Caelo	Lactato de cálcio penta-h…	23002025	26971SI	20	20230918*
Fagron	Lactato de cálcio penta-h…	12E10-N03	20745	40	20120704
Fagron	Lactato de cálcio penta-h…	12I12-N06	21232	40	AR-15-FG-007939-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Lactato de cálcio penta-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Lactato de cálcio penta-hidratado*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lactato de cálcio penta-h…	171377	23642	40
Caelo	Lactato de cálcio penta-h…	180734	24035	40
Caelo	Lactato de cálcio penta-h…	24002487	27428	40
Fagron	Lactato de cálcio penta-h…	14H01-B05-323830	23566	40
Fagron	Lactato de cálcio penta-h…	23C16-B11-234646	27036	40
Caelo	Lactato de cálcio penta-h…	24002487	27428SI	20
Fagron	Lactato de cálcio penta-h…	23C16-B11-234646	27036SI	20

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 79 spectra from 38 *Apo-Ident* customers from 48 batches from the substance/substance group *Lactato de cálcio penta-hidratado*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Lactato de cálcio penta-h…	11369606	1
Caelo	Lactato de cálcio penta-h…	11369610	1
Caelo	Lactato de cálcio penta-h…	11369614	2
Caelo	Lactato de cálcio penta-h…	11369618	1
Caelo	Lactato de cálcio penta-h…	12C15-N02	1
Caelo	Lactato de cálcio penta-h…	12E10-N03	1
Caelo	Lactato de cálcio penta-h…	13080802	2
Caelo	Lactato de cálcio penta-h…	13080804	2
Caelo	Lactato de cálcio penta-h…	13080805	2
Caelo	Lactato de cálcio penta-h…	14H01B05300502	1
Caelo	Lactato de cálcio penta-h…	15101409	1
Caelo	Lactato de cálcio penta-h…	15101411	2
Caelo	Lactato de cálcio penta-h…	15101412	3
Caelo	Lactato de cálcio penta-h…	15227804	2
Caelo	Lactato de cálcio penta-h…	16131302	1
Caelo	Lactato de cálcio penta-h…	16131307	1
Caelo	Lactato de cálcio penta-h…	16131312	1
Caelo	Lactato de cálcio penta-h…	16333106	4
Caelo	Lactato de cálcio penta-h…	16333111	4
Caelo	Lactato de cálcio penta-h…	16333113	1
Caelo	Lactato de cálcio penta-h…	17137707	2
Caelo	Lactato de cálcio penta-h…	17355503	2
Caelo	Lactato de cálcio penta-h…	17J18-B01-350892	1
Caelo	Lactato de cálcio penta-h…	18073406	2
Caelo	Lactato de cálcio penta-h…	18073413	2
Caelo	Lactato de cálcio penta-h…	18073415	2
Caelo	Lactato de cálcio penta-h…	19042208	1
Caelo	Lactato de cálcio penta-h…	20000512004	1
Caelo	Lactato de cálcio penta-h…	20003749002	1
Caelo	Lactato de cálcio penta-h…	20003749008	1
Caesar & Loretz GmbH	Lactato de cálcio penta-h…	19042203	2
Fagron	Lactato de cálcio penta-h…	12/12-N06	1
Fagron	Lactato de cálcio penta-h…	12C15-N02	1
Fagron	Lactato de cálcio penta-h…	12I12-N01	1
Fagron	Lactato de cálcio penta-h…	12I12-N06	2
Fagron	Lactato de cálcio penta-h…	13L18B04	1
Fagron	Lactato de cálcio penta-h…	13L18-B04-295541	3
Fagron	Lactato de cálcio penta-h…	14H01-B05	1
Fagron	Lactato de cálcio penta-h…	14H01-B05-334588	2
Fagron	Lactato de cálcio penta-h…	17J18-B01-343387	1
Fagron	Lactato de cálcio penta-h…	17J18-B01-347174	1
Fagron	Lactato de cálcio penta-h…	1806000537	1
Fagron	Lactato de cálcio penta-h…	1901001645	1
Fagron	Lactato de cálcio penta-h…	19B26-B05	1
Fagron	Lactato de cálcio penta-h…	20C31-B02-201355	2
Fagron	Lactato de cálcio penta-h…	21B23-B02-210092	2
Fagron	Lactato de cálcio penta-h…	21B23-BO2-210092	1
Fagron	Lactato de cálcio penta-h…	21F09-B02-215877	3
Phönix	Lactato de cálcio penta-h…	14H01-B05	1
phönix	Lactato de cálcio penta-h…	15101411	1
Shop	Lactato de cálcio penta-h…	1111001829	1

- 235 988 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Lactato de cálcio penta-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lactato de cálcio penta-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	240	0	201 844
Type C	0	79	0	235 988

The substance/substance group *Lactato de cálcio penta-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.4051 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20745	22445	7,66	139,53
21232	21232	0,00	136,66
21909	22445	8,28	141,22
22263	22445	6,68	139,14
22445	22445	0,00	141,91
25225	25225	0,00	137,58
26971	26971	0,00	144,12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lactato de etacridina monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20750-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lactato de etacridina monoidratado; Ethacridini lactas monohydricus

Special notes

When selecting the *Lactato de etacridina monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lactato de etacridina monoidratado	7	5	94

Second-stage model

For differentiation of the substance/substance group *Lactato de etacridina monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lactato de etacridina monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	76,59	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lactato de etacridina monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lactato de etacridina monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lactato de etacridina mon…	12149507	20750	40	20120619
Caelo	Lactato de etacridina mon…	16273403	23247	40	20161122
Caelo	Lactato de etacridina mon…	22001737	26357	40	20220819*
Euro OTC	Lactato de etacridina mon…	1206016-02	21636	60	20121019
Euro OTC	Lactato de etacridina mon…	1412034-02	22733	40	20150223
Fagron	Lactato de etacridina mon…	13I24-N03	21265	40	AR-15-FG-007011-02
Fagron	Lactato de etacridina mon…	15A29-B02-306219	22500	40	20150205

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Lactato de etacridina monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 9 reference samples from the substance/substance group *Lactato de etacridina monoidratado*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lactato de etacridina mon…	172476	23671	40
Caelo	Lactato de etacridina mon…	183146	24355	40
Caelo	Lactato de etacridina mon…	20001048	25203	40
Caelo	Lactato de etacridina mon…	21001424012	25925	40
Fagron	Lactato de etacridina mon…	21C17-B01-215098	26065	40
Caelo	Lactato de etacridina mon…	172476	23798	40
Caelo	Lactato de etacridina mon…	21001424012	25925SI	10
Caelo	Lactato de etacridina mon…	22001737	26357SI†	20
Fagron	Lactato de etacridina mon…	21C17-B01-215098	26065SI	10

- 201 804 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 451 spectra from 270 *Apo-Ident* customers from 101 batches from the substance/substance group *Lactato de etacridina monoidratado*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 94 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lactato de etacridina mon…	22001737005	1
	Lactato de etacridina mon…	22001737011	2
AHD	Lactato de etacridina mon…	22001737016	1
AHL	Lactato de etacridina mon…	141101	1
Alliance Healthcare	Lactato de etacridina mon…	141234-04	1
Anzag	Lactato de etacridina mon…	111201	1
Anzag	Lactato de etacridina mon…	18314601	1
Bombastus	Lactato de etacridina mon…	13/24-N03	1
Bombastus	Lactato de etacridina mon…	14A15-B04-300493	1
cae	Lactato de etacridina mon…	16272410	1
cae	Lactato de etacridina mon…	20004177003	1
Caelo	Lactato de etacridina mon…	10288702	1
Caelo	Lactato de etacridina mon…	11J07-N05	1
Caelo	Lactato de etacridina mon…	1206016-03	1
Caelo	Lactato de etacridina mon…	12149507	3
Caelo	Lactato de etacridina mon…	12268407	3
Caelo	Lactato de etacridina mon…	12G02-N13	2
Caelo	Lactato de etacridina mon…	141203401	1
Caelo	Lactato de etacridina mon…	1412034-01	1
Caelo	Lactato de etacridina mon…	1412034-02	1
Caelo	Lactato de etacridina mon…	1412034-03	2
Caelo	Lactato de etacridina mon…	141203404	1
Caelo	Lactato de etacridina mon…	1412034-04	2
Caelo	Lactato de etacridina mon…	15/214/R	1
Caelo	Lactato de etacridina mon…	15177603	4
Caelo	Lactato de etacridina mon…	15177608	2
Caelo	Lactato de etacridina mon…	15177612	1
Caelo	Lactato de etacridina mon…	15438003	6
Caelo	Lactato de etacridina mon…	15438007	4
Caelo	Lactato de etacridina mon…	15438009	2
Caelo	Lactato de etacridina mon…	16272401	1
Caelo	Lactato de etacridina mon…	16272406	1
Caelo	Lactato de etacridina mon…	16272408	3
Caelo	Lactato de etacridina mon…	16272410	3
Caelo	Lactato de etacridina mon…	16272412	1
Caelo	Lactato de etacridina mon…	16272413	1
Caelo	Lactato de etacridina mon…	162734	1
Caelo	Lactato de etacridina mon…	16273403	8
Caelo	Lactato de etacridina mon…	16273411	9
Caelo	Lactato de etacridina mon…	1627412	1
Caelo	Lactato de etacridina mon…	17247605	14
Caelo	Lactato de etacridina mon…	17247606	1
Caelo	Lactato de etacridina mon…	17332303	4
Caelo	Lactato de etacridina mon…	17332304	16
Caelo	Lactato de etacridina mon…	17332312	4
Caelo	Lactato de etacridina mon…	17332314	12
Caelo	Lactato de etacridina mon…	17332316	6
Caelo	Lactato de etacridina mon…	1814607	1
Caelo	Lactato de etacridina mon…	183146004	4
Caelo	Lactato de etacridina mon…	183146005	6
Caelo	Lactato de etacridina mon…	18314601	9
Caelo	Lactato de etacridina mon…	18314603	1
Caelo	Lactato de etacridina mon…	18314605	1
Caelo	Lactato de etacridina mon…	18314607	27
Caelo	Lactato de etacridina mon…	18314608	1
Caelo	Lactato de etacridina mon…	20001048002	9
Caelo	Lactato de etacridina mon…	20001048004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactato de etacridina mon…	20004177003	10
Caelo	Lactato de etacridina mon…	21001424004	13
Caelo	Lactato de etacridina mon…	21001424012	1
Caelo	Lactato de etacridina mon…	21001424013	1
Caelo	Lactato de etacridina mon…	21001424014	5
Caelo	Lactato de etacridina mon…	22001737003	7
Caelo	Lactato de etacridina mon…	22001737008	1
Caelo	Lactato de etacridina mon…	22001737011	1
Caelo	Lactato de etacridina mon…	22001737013	1
Caelo	Lactato de etacridina mon…	2201737003	1
Caelo	Lactato de etacridina mon…	7247805	1
Caesar & Lorenz GmbH	Lactato de etacridina mon…	18314601	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	18314601	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	17332304	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	17332314	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	18314601	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	20004177003	1
Caesar & Loretz GmbH/AHD	Lactato de etacridina mon…	20001048002	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	22001737003	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	17332316	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	20001048002	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	18314607	1
Caesar & Loretz GmbH/Kehr	Lactato de etacridina mon…	21001424004	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	22001737003	1
Caesar & Loretz GmbH…	Lactato de etacridina mon…	20001048	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	17332314	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	183146002	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	183146005	3
Caesar & Loretz GmbH	Lactato de etacridina mon…	18314601	3
Caesar & Loretz GmbH	Lactato de etacridina mon…	18314607	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	20001048002	4
Caesar & Loretz GmbH	Lactato de etacridina mon…	20001048003	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	20001048006	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	20004177003	2
Caesar & Loretz GmbH	Lactato de etacridina mon…	21001424004	2
Caesar & Loretz GmbH	Lactato de etacridina mon…	21001424012	2
Caesar & Loretz GmbH	Lactato de etacridina mon…	21001424013	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	22001737008	1
Caesar & Loretz GmbH	Lactato de etacridina mon…	caelo	1
Caesar & Loretz/Gehe	Lactato de etacridina mon…	20001048002	1
Caleo/ Noweda	Lactato de etacridina mon…	17332312	1
Cealo/Sanacorp	Lactato de etacridina mon…	21001424013	1
Chinosol/Anzag	Lactato de etacridina mon…	2112A-02196	1
Chinosol/Anzag	Lactato de etacridina mon…	914E-02196	1
Dermapharm	Lactato de etacridina mon…	100201	1
Dermapharm	Lactato de etacridina mon…	111201	5
Dermapharm	Lactato de etacridina mon…	130201	8
Dermapharm	Lactato de etacridina mon…	141101	11
Dermopharm	Lactato de etacridina mon…	130201	1
Dermopharm	Lactato de etacridina mon…	141101	1
E Plus	Lactato de etacridina mon…	17332314	1
Ebert & Jacobi 19…	Lactato de etacridina mon…	141101	2
Ebert & Jacobi	Lactato de etacridina mon…	15177608	1
Euro OTC	Lactato de etacridina mon…	1206016-02	4
Euro OTC	Lactato de etacridina mon…	1206016-03	6
Euro OTC	Lactato de etacridina mon…	13/24-N03	1
Euro OTC	Lactato de etacridina mon…	1412034-01	5
Euro OTC	Lactato de etacridina mon…	1412034-02	2
Euro OTC	Lactato de etacridina mon…	1412034-03	13
Euro OTC	Lactato de etacridina mon…	141203404	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Lactato de etacridina mon…	1412034-04	4
Euro OTC	Lactato de etacridina mon…	15438007	1
Euro OTC	Lactato de etacridina mon…	17332304	2
Euro OTC	Lactato de etacridina mon…	1807013-01	9
Euro OTC	Lactato de etacridina mon…	1807013-02	4
Euro OTC	Lactato de etacridina mon…	20001048002	1
Euro OTC	Lactato de etacridina mon…	2905007-01	1
Euro OTC	Lactato de etacridina mon…	2905007v-03	1
Euro OTC	Lactato de etacridina mon…	2905007V-03	1
Euro OTC	Lactato de etacridina mon…	A201801002	1
Fagron	Lactato de etacridina mon…	11/07-N05	1
Fagron	Lactato de etacridina mon…	12/24-N04	2
Fagron	Lactato de etacridina mon…	12324N03	1
Fagron	Lactato de etacridina mon…	12A02-N10	1
Fagron	Lactato de etacridina mon…	12C30-N07	1
Fagron	Lactato de etacridina mon…	12G02-N13	5
Fagron	Lactato de etacridina mon…	12G02-N135-15	1
Fagron	Lactato de etacridina mon…	12J24-N04	1
Fagron	Lactato de etacridina mon…	13/24-N03	5
Fagron	Lactato de etacridina mon…	13/24-NO3	1
Fagron	Lactato de etacridina mon…	13I24-N03	7
Fagron	Lactato de etacridina mon…	13l24-N03	1
Fagron	Lactato de etacridina mon…	1412034-04	1
Fagron	Lactato de etacridina mon…	14A15-B04	2
Fagron	Lactato de etacridina mon…	14A15-B04-300493	6
Fagron	Lactato de etacridina mon…	16273411	1
Fagron	Lactato de etacridina mon…	16e20-b11-322514	1
Fagron	Lactato de etacridina mon…	16E20-B11-322514	5
Fagron	Lactato de etacridina mon…	16E20-B11-326633	1
Fagron	Lactato de etacridina mon…	16E20-B11-328430	1
Fagron	Lactato de etacridina mon…	201205001	2
Finze	Lactato de etacridina mon…	90601	1
Gehe amax	Lactato de etacridina mon…	18314607	1
Gehe	Lactato de etacridina mon…	13I24-N03	1
Gehe	Lactato de etacridina mon…	141101	1
Gehe	Lactato de etacridina mon…	1412034-03	1
Gehe	Lactato de etacridina mon…	17247605	2
Gehe	Lactato de etacridina mon…	21001424014	1
Gehe	Lactato de etacridina mon…	22001737008	1
Kehr	Lactato de etacridina mon…	22001737014	1
Kehr	Lactato de etacridina mon…	22001737016	1
Liaoyuang Silver Eag…	Lactato de etacridina mon…	1412034-02	1
Noweda	Lactato de etacridina mon…	183146005	1
Noweda	Lactato de etacridina mon…	18314601	1
Noweda	Lactato de etacridina mon…	18314607	2
Noweda	Lactato de etacridina mon…	20001048002	2
Noweda	Lactato de etacridina mon…	22001737011	3
Noweda	Lactato de etacridina mon…	3785846	1
phoenix 18.11.2014	Lactato de etacridina mon…	13/24-N03	1
Phoenix	Lactato de etacridina mon…	100201	1
Phoenix	Lactato de etacridina mon…	1412034-03	1
Phoenix	Lactato de etacridina mon…	22001737016	1
Phönix	Lactato de etacridina mon…	111201	1
Phonix	Lactato de etacridina mon…	13I24-N03	1
Phönix	Lactato de etacridina mon…	20001048002	1
Rezepturlager - Verl…	Lactato de etacridina mon…	121/15	1
Rezepturlager - Verl…	Lactato de etacridina mon…	220/17	1
Sanacorp HST	Lactato de etacridina mon…	17247605	1
Sanacorp/EuRho	Lactato de etacridina mon…	1412034-03	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 616 spectra from 1515 *Apo-Ident* customers from a total of 49 159 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lactato de etacridina monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lactato de etacridina monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	280	0	201 804
Type C	0	445	6	235 616

The substance/substance group *Lactato de etacridina monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	98.6696 % (> 98.0044 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20750	21265	6,17	150,05
21265	21265	0,00	148,28
21636	21265	8,45	151,69
22500	21265	11,34	149,47
22733	21265	12,84	148,32
23247	21265	11,95	150,01
26357	26357	0,00	159,60

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lactose monoidratada**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20029-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lactose monoidratada; Lactosum monohydricum

Special notes

When selecting the *Lactose monoidratada* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lactose monoidratada	6	14	521

Second-stage model

For differentiation of the substance/substance group *Lactose monoidratada* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lactose monoidratada* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Pancreatina, pulverizada	35,41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lactose monoidratada* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lactose monoidratada*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lactose monoidratada	12139910	20685	30	20120606
Caelo	Lactose monoidratada	14025601	21525	40	20140207
Caelo	Lactose monoidratada	14025601	21526	40	20140207
Caelo	Lactose monoidratada	14025601	21527	40	20140207
Caelo	Lactose monoidratada	14025601	21528	40	20140207
Caelo	Lactose monoidratada	14025601	21529	40	20140207
Caelo	Lactose monoidratada	160277	22460	60	20160321*
Euro OTC	Lactose monoidratada	1509030	21935	60	20151013*
Euro OTC	Lactose monoidratada	1606025	22701	40	20160628*
Euro OTC	Lactose monoidratada	1909014	24929	40	20191015*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 430 spectra of 10 reference samples from the substance/substance group *Lactose monoidratada*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 532 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 17 reference samples from the substance/substance group *Lactose monoidratada*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lactose monoidratada	15236220	22584	40
Caelo	Lactose monoidratada	173360	23828	40
Caelo	Lactose monoidratada	192364	25233	40
Caelo	Lactose monoidratada	191376	25234	40
Caelo	Lactose monoidratada	21001507	25804	50
Caelo	Lactose monoidratada	23001015	26694	40
Caelo	Lactose monoidratada	24001886	27332	40
Euro OTC	Lactose monoidratada	1703019	23141	40
Euro OTC	Lactose monoidratada	1802002	23962	40
Euro OTC	Lactose monoidratada	1812008	24415	40
Euro OTC	Lactose monoidratada	2005026	25275	40
Euro OTC	Lactose monoidratada	2201013	25952	40
Euro OTC	Lactose monoidratada	2208008	26277	40
Euro OTC	Lactose monoidratada	2309012	27012	40
Caelo	Lactose monoidratada	23001015	26694SI	20
Euro OTC	Lactose monoidratada	2201013	25952SI	10
Euro OTC	Lactose monoidratada	2208008	26277SI	20

- 201 464 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2465 spectra from 667 *Apo-Ident* customers from 526 batches from the substance/substance group *Lactose monoidratada*.

- Among them are spectra of independent samples from 521 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lactose monoidratada	14025604	1
	Lactose monoidratada	2005026-02	1
	Lactose monoidratada	22000736005	1
	Lactose monoidratada	22000736007	1
	Lactose monoidratada	22000736008	3
	Lactose monoidratada	22000736010	1
	Lactose monoidratada	22000736012	1
	Lactose monoidratada	22000736016	2
	Lactose monoidratada	22000736018	3
	Lactose monoidratada	2208008-01	1
	Lactose monoidratada	2208008-02	1
	Lactose monoidratada	2208008-03	3
	Lactose monoidratada	23001015001	4
	Lactose monoidratada	23001015003	13
	Lactose monoidratada	23001015004	11
	Lactose monoidratada	23001015007	3
	Lactose monoidratada	23002236002	11
	Lactose monoidratada	23002236003	8
	Lactose monoidratada	23002236005	2
	Lactose monoidratada	23003217001	4
	Lactose monoidratada	23003217003	4
	Lactose monoidratada	23003217009	1
	Lactose monoidratada	2309012-01	2
	Lactose monoidratada	309351/0	1
	Lactose monoidratada	309508/0	1
A.H.D.	Lactose monoidratada	12336801	1
AEP	Lactose monoidratada	18198007	2
AHD	Lactose monoidratada	13I23-B03-291114	1
AHD	Lactose monoidratada	15236220	1
AHD	Lactose monoidratada	192364002	1
AHD	Lactose monoidratada	22000736017	1
AHD	Lactose monoidratada	23001015001	1
AHD	Lactose monoidratada	23003217005	1
Alliance H.	Lactose monoidratada	C12H22011	1
Alliance Healthcare	Lactose monoidratada	10195101	2
Alliance Healthcare	Lactose monoidratada	22000736005	1
Alliance	Lactose monoidratada	20004200007	1
Alliance	Lactose monoidratada	22000736018	4
Alliance	Lactose monoidratada	23001015003	1
Alliance	Lactose monoidratada	23003217004	1
Alliance	Lactose monoidratada	23003217009	1
Alte Apotheke	Lactose monoidratada	16027708	1
Anzag / Noweda	Lactose monoidratada	12336815	1
Anzag 29.11.12 ek:7,51	Lactose monoidratada	12139914	1
Anzag/Fragon	Lactose monoidratada	1005SLP	1
Anzag	Lactose monoidratada	12139915	5
Anzag	Lactose monoidratada	192364014	1
api-ident	Lactose monoidratada	17078312	1
Bahnhof-Apotheke	Lactose monoidratada	120614	1
Bahnhof-Apotheke	Lactose monoidratada	120808	1
Bahnhof-Apotheke	Lactose monoidratada	121119	2
Bahnhof-Apotheke	Lactose monoidratada	130115	1
Bahnhof-Apotheke	Lactose monoidratada	130729	1
Bahnhof-Apotheke	Lactose monoidratada	130911	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bahnhof-Apotheke	Lactose monoidratada	130925	1
Bahnhof-Apotheke	Lactose monoidratada	131023	1
Bahnhof-Apotheke	Lactose monoidratada	131112	1
Bahnhof-Apotheke	Lactose monoidratada	131127	2
Bahnhof-Apotheke	Lactose monoidratada	131218	2
Bahnhof-Apotheke	Lactose monoidratada	140113	3
Bahnhof-Apotheke	Lactose monoidratada	140206	2
Bahnhof-Apotheke	Lactose monoidratada	140220	1
Bahnhof-Apotheke	Lactose monoidratada	140310	2
Bahnhof-Apotheke	Lactose monoidratada	140630	1
Bahnhofsapotheke	Lactose monoidratada	140401	1
Bären Apotheke	Lactose monoidratada	16231206	1
Bombastus	Lactose monoidratada	13299108	1
Bombastus	Lactose monoidratada	17000754	1
Bombastus	Lactose monoidratada	17001199	1
Bombastus	Lactose monoidratada	17001212	1
Bombastus	Lactose monoidratada	17078302	1
Bombastus	Lactose monoidratada	272680/0	1
Bombastus	Lactose monoidratada	274926	1
Bombastus	Lactose monoidratada	275194/0	1
Bombastus	Lactose monoidratada	275225/0	1
Bombastus	Lactose monoidratada	282648	1
Bombastus	Lactose monoidratada	282696/0	1
Bombastus	Lactose monoidratada	283992	2
Bombastus	Lactose monoidratada	284321/0	1
Bombastus	Lactose monoidratada	285087/0	1
Bombastus	Lactose monoidratada	286354	1
Bombastus	Lactose monoidratada	286697/0	1
Bombastus	Lactose monoidratada	286710	1
Bombastus	Lactose monoidratada	288015/0	1
Bombastus	Lactose monoidratada	288927	1
Bombastus	Lactose monoidratada	289238	1
Bombastus	Lactose monoidratada	291464	1
Bombastus	Lactose monoidratada	292982	2
Bombastus	Lactose monoidratada	292983	1
Bombastus	Lactose monoidratada	292995	1
Bombastus	Lactose monoidratada	292996	1
Bombastus	Lactose monoidratada	293074	1
Bombastus	Lactose monoidratada	2932880	1
Bombastus	Lactose monoidratada	293289	1
Bombastus	Lactose monoidratada	293290	1
Bombastus	Lactose monoidratada	293649	1
Bombastus	Lactose monoidratada	293918/0	1
Bombastus	Lactose monoidratada	293970	1
Bombastus	Lactose monoidratada	294154	1
Bombastus	Lactose monoidratada	294184/0	1
Bombastus	Lactose monoidratada	294897/0	1
Bombastus	Lactose monoidratada	295011/0	1
Bombastus	Lactose monoidratada	295476	1
Bombastus	Lactose monoidratada	295714	1
Bombastus	Lactose monoidratada	295715	1
Bombastus	Lactose monoidratada	300657	2
Bombastus	Lactose monoidratada	3020165	1
Bombastus	Lactose monoidratada	303658	2
Bombastus	Lactose monoidratada	304755	1
Bombastus	Lactose monoidratada	305227	2
Bombastus	Lactose monoidratada	305227/0	1
Bombastus	Lactose monoidratada	305336	2
Bombastus	Lactose monoidratada	305336/0	1
Bombastus	Lactose monoidratada	306147	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Lactose monoidratada	306651/0	1
Bombastus	Lactose monoidratada	306652	1
Bombastus	Lactose monoidratada	306850	1
Bombastus	Lactose monoidratada	306964	1
Bombastus	Lactose monoidratada	306989	2
Bombastus	Lactose monoidratada	306990	1
Bombastus	Lactose monoidratada	307444/0	1
Bombastus	Lactose monoidratada	307543	2
Bombastus	Lactose monoidratada	307573/0	1
Bombastus	Lactose monoidratada	307702/0	1
Bombastus	Lactose monoidratada	307741	1
Bombastus	Lactose monoidratada	3077410	1
Bombastus	Lactose monoidratada	307976/0	1
Bombastus	Lactose monoidratada	308117	1
Bombastus	Lactose monoidratada	308117/0	1
Bombastus	Lactose monoidratada	308118/0	1
Bombastus	Lactose monoidratada	308438	1
Bombastus	Lactose monoidratada	309351	1
Bombastus	Lactose monoidratada	309413/0	1
Bombastus	Lactose monoidratada	309508	1
Bombastus	Lactose monoidratada	309509	1
Bombastus	Lactose monoidratada	309509/0	1
Bombastus	Lactose monoidratada	310082/0	1
Bombastus	Lactose monoidratada	310691	1
Bombastus	Lactose monoidratada	310691/0	1
Bombastus	Lactose monoidratada	310905	1
Bombastus	Lactose monoidratada	310905/0	1
Bombastus	Lactose monoidratada	310912/0	1
Bombastus	Lactose monoidratada	311280	1
Bombastus	Lactose monoidratada	311280/0	1
Bombastus	Lactose monoidratada	311362/0	1
C21001507004aelo/Gehe	Lactose monoidratada	21001507004	1
Caelo	Lactose monoidratada		3
Caelo	Lactose monoidratada	10071701	1
Caelo	Lactose monoidratada	10195107	2
Caelo	Lactose monoidratada	1071302	1
Caelo	Lactose monoidratada	1090216	1
Caelo	Lactose monoidratada	11014714	1
Caelo	Lactose monoidratada	11041801	1
Caelo	Lactose monoidratada	1106022-02	1
Caelo	Lactose monoidratada	11079002	2
Caelo	Lactose monoidratada	112192	2
Caelo	Lactose monoidratada	11219207	1
Caelo	Lactose monoidratada	11219208	3
Caelo	Lactose monoidratada	11219216	2
Caelo	Lactose monoidratada	12021502	1
Caelo	Lactose monoidratada	12021508	1
Caelo	Lactose monoidratada	12021518	5
Caelo	Lactose monoidratada	12041401	1
Caelo	Lactose monoidratada	12139901	2
Caelo	Lactose monoidratada	12139908	1
Caelo	Lactose monoidratada	12139909	1
Caelo	Lactose monoidratada	12139910	1
Caelo	Lactose monoidratada	12139912	1
Caelo	Lactose monoidratada	12139914	6
Caelo	Lactose monoidratada	12139915	4
Caelo	Lactose monoidratada	12139920	6
Caelo	Lactose monoidratada	12336801	7
Caelo	Lactose monoidratada	12336814	1
Caelo	Lactose monoidratada	12336815	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monoidratada	12336816	3
Caelo	Lactose monoidratada	12336820	2
Caelo	Lactose monoidratada	123446test	1
Caelo	Lactose monoidratada	123456	1
Caelo	Lactose monoidratada	123456test	1
Caelo	Lactose monoidratada	12345test	1
Caelo	Lactose monoidratada	1234test	1
Caelo	Lactose monoidratada	12399107	1
Caelo	Lactose monoidratada	123test	6
Caelo	Lactose monoidratada	123Test	4
Caelo	Lactose monoidratada	1301C005	2
Caelo	Lactose monoidratada	13081302	1
Caelo	Lactose monoidratada	13104901	5
Caelo	Lactose monoidratada	13104902	7
Caelo	Lactose monoidratada	13104908	2
Caelo	Lactose monoidratada	13104909	5
Caelo	Lactose monoidratada	13104909-3422310182	1
Caelo	Lactose monoidratada	13104909-3453311172	1
Caelo	Lactose monoidratada	13104910	2
Caelo	Lactose monoidratada	13104911	2
Caelo	Lactose monoidratada	13104912	1
Caelo	Lactose monoidratada	13299101	9
Caelo	Lactose monoidratada	13299102	12
Caelo	Lactose monoidratada	13299103	1
Caelo	Lactose monoidratada	13299107	5
Caelo	Lactose monoidratada	13299108	5
Caelo	Lactose monoidratada	1401003-01	1
Caelo	Lactose monoidratada	1402504	1
Caelo	Lactose monoidratada	14025601	3
Caelo	Lactose monoidratada	14025603	7
Caelo	Lactose monoidratada	14025604	6
Caelo	Lactose monoidratada	14025608	2
Caelo	Lactose monoidratada	14025615	1
Caelo	Lactose monoidratada	14025616	4
Caelo	Lactose monoidratada	14025619	3
Caelo	Lactose monoidratada	14025620	15
Caelo	Lactose monoidratada	140612	3
Caelo	Lactose monoidratada	14140302	4
Caelo	Lactose monoidratada	14140304	2
Caelo	Lactose monoidratada	14140305	8
Caelo	Lactose monoidratada	14140308	7
Caelo	Lactose monoidratada	14140309	2
Caelo	Lactose monoidratada	14140312	14
Caelo	Lactose monoidratada	14333501	3
Caelo	Lactose monoidratada	14333502	2
Caelo	Lactose monoidratada	14333503	1
Caelo	Lactose monoidratada	14333508	1
Caelo	Lactose monoidratada	14333509	10
Caelo	Lactose monoidratada	14333510	1
Caelo	Lactose monoidratada	14333511	5
Caelo	Lactose monoidratada	143335114	1
Caelo	Lactose monoidratada	14333513	7
Caelo	Lactose monoidratada	14333514	1
Caelo	Lactose monoidratada	14333518	4
Caelo	Lactose monoidratada	14333520	10
Caelo	Lactose monoidratada	14333521	8
Caelo	Lactose monoidratada	14333525	1
Caelo	Lactose monoidratada	14333528	2
Caelo	Lactose monoidratada	1433502	1
Caelo	Lactose monoidratada	1433510	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monoidratada	1433518	2
Caelo	Lactose monoidratada	1433520	1
Caelo	Lactose monoidratada	1433521	1
Caelo	Lactose monoidratada	1501017-01	4
Caelo	Lactose monoidratada	15011701	1
Caelo	Lactose monoidratada	15081701	1
Caelo	Lactose monoidratada	150903002	1
Caelo	Lactose monoidratada	1509030-02	1
Caelo	Lactose monoidratada	1523614	1
Caelo	Lactose monoidratada	152362	2
Caelo	Lactose monoidratada	15236201	28
Caelo	Lactose monoidratada	15236202	1
Caelo	Lactose monoidratada	15236203	4
Caelo	Lactose monoidratada	15236204	11
Caelo	Lactose monoidratada	15236206	1
Caelo	Lactose monoidratada	15236208	13
Caelo	Lactose monoidratada	15236209	12
Caelo	Lactose monoidratada	15236209I-060616/1	1
Caelo	Lactose monoidratada	15236213	2
Caelo	Lactose monoidratada	15236214	9
Caelo	Lactose monoidratada	15236215	4
Caelo	Lactose monoidratada	15236217	1
Caelo	Lactose monoidratada	15236220	5
Caelo	Lactose monoidratada	15236221	7
Caelo	Lactose monoidratada	1526201	1
Caelo	Lactose monoidratada	1565555	1
Caelo	Lactose monoidratada	16027701	6
Caelo	Lactose monoidratada	16027702	9
Caelo	Lactose monoidratada	16027703	6
Caelo	Lactose monoidratada	16027704	3
Caelo	Lactose monoidratada	16027705	1
Caelo	Lactose monoidratada	16027706	7
Caelo	Lactose monoidratada	16027707	2
Caelo	Lactose monoidratada	16027708	11
Caelo	Lactose monoidratada	16027726	1
Caelo	Lactose monoidratada	1606025-01	4
Caelo	Lactose monoidratada	1606025-1	1
Caelo	Lactose monoidratada	160913PJK01	1
Caelo	Lactose monoidratada	16091710	1
Caelo	Lactose monoidratada	162310206	1
Caelo	Lactose monoidratada	16231201	10
Caelo	Lactose monoidratada	16231202	20
Caelo	Lactose monoidratada	16231203	4
Caelo	Lactose monoidratada	16231206	7
Caelo	Lactose monoidratada	16231207	11
Caelo	Lactose monoidratada	16231208	5
Caelo	Lactose monoidratada	1623120803815470	1
Caelo	Lactose monoidratada	16231211	27
Caelo	Lactose monoidratada	16231212	10
Caelo	Lactose monoidratada	16231213	4
Caelo	Lactose monoidratada	162312135465	1
Caelo	Lactose monoidratada	16231214	5
Caelo	Lactose monoidratada	16231215	5
Caelo	Lactose monoidratada	16321202	1
Caelo	Lactose monoidratada	17011301	1
Caelo	Lactose monoidratada	1703019-01	3
Caelo	Lactose monoidratada	1703019-020	1
Caelo	Lactose monoidratada	17078302	11
Caelo	Lactose monoidratada	17078303	39
Caelo	Lactose monoidratada	17078303-20180619Ma2	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monoidratada	17078306	11
Caelo	Lactose monoidratada	17078307	8
Caelo	Lactose monoidratada	17078312	25
Caelo	Lactose monoidratada	17321001	38
Caelo	Lactose monoidratada	173210016	1
Caelo	Lactose monoidratada	17321002	4
Caelo	Lactose monoidratada	17321004	9
Caelo	Lactose monoidratada	17321005	4
Caelo	Lactose monoidratada	17321006	1
Caelo	Lactose monoidratada	1733008	1
Caelo	Lactose monoidratada	17336001	1
Caelo	Lactose monoidratada	17336002	16
Caelo	Lactose monoidratada	17336005	12
Caelo	Lactose monoidratada	17336007	47
Caelo	Lactose monoidratada	17336008	20
Caelo	Lactose monoidratada	17336009	11
Caelo	Lactose monoidratada	17336013	20
Caelo	Lactose monoidratada	17336014	14
Caelo	Lactose monoidratada	1733609	1
Caelo	Lactose monoidratada	1802002-01	1
Caelo	Lactose monoidratada	18169016P-191115-2	1
Caelo	Lactose monoidratada	1818003	1
Caelo	Lactose monoidratada	18192001	1
Caelo	Lactose monoidratada	18196004	1
Caelo	Lactose monoidratada	18196023	2
Caelo	Lactose monoidratada	18198001	20
Caelo	Lactose monoidratada	18198002	6
Caelo	Lactose monoidratada	18198003	4
Caelo	Lactose monoidratada	18198005	1
Caelo	Lactose monoidratada	18198006	18
Caelo	Lactose monoidratada	18198007	24
Caelo	Lactose monoidratada	18198008	4
Caelo	Lactose monoidratada	18198009	1
Caelo	Lactose monoidratada	18198013	13
Caelo	Lactose monoidratada	18198014	11
Caelo	Lactose monoidratada	18198015	2
Caelo	Lactose monoidratada	18198016	24
Caelo	Lactose monoidratada	18198016P-191227-1	1
Caelo	Lactose monoidratada	18198017	9
Caelo	Lactose monoidratada	18198018	9
Caelo	Lactose monoidratada	18198023	22
Caelo	Lactose monoidratada	19137601	19
Caelo	Lactose monoidratada	19137601P-200303-1	1
Caelo	Lactose monoidratada	19137601P-200612-1	1
Caelo	Lactose monoidratada	19137602	7
Caelo	Lactose monoidratada	1922364001	1
Caelo	Lactose monoidratada	192346002	1
Caelo	Lactose monoidratada	192354015	1
Caelo	Lactose monoidratada	19236009	1
Caelo	Lactose monoidratada	192364001	6
Caelo	Lactose monoidratada	192364002	17
Caelo	Lactose monoidratada	192364003	13
Caelo	Lactose monoidratada	192364008	5
Caelo	Lactose monoidratada	192364009	14
Caelo	Lactose monoidratada	192364011	27
Caelo	Lactose monoidratada	192364012	18
Caelo	Lactose monoidratada	192364014	9
Caelo	Lactose monoidratada	192364015	16
Caelo	Lactose monoidratada	192364016	4
Caelo	Lactose monoidratada	19236403	30

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monoidratada	2000400007	1
Caelo	Lactose monoidratada	20004200001	6
Caelo	Lactose monoidratada	20004200003	1
Caelo	Lactose monoidratada	20004200004	20
Caelo	Lactose monoidratada	20004200005	9
Caelo	Lactose monoidratada	20004200006	6
Caelo	Lactose monoidratada	20004200007	4
Caelo	Lactose monoidratada	20004200009	6
Caelo	Lactose monoidratada	2000420004	3
Caelo	Lactose monoidratada	2000420005	1
Caelo	Lactose monoidratada	20021411	1
Caelo	Lactose monoidratada	200415HJK02	1
Caelo	Lactose monoidratada	2011901	1
Caelo	Lactose monoidratada	201910028	1
Caelo	Lactose monoidratada	20223445	1
Caelo	Lactose monoidratada	2051702	1
Caelo	Lactose monoidratada	21001507003	13
Caelo	Lactose monoidratada	21001507004	13
Caelo	Lactose monoidratada	21001507005	4
Caelo	Lactose monoidratada	21001507008	2
Caelo	Lactose monoidratada	2100843006	1
Caelo	Lactose monoidratada	21071801	1
Caelo	Lactose monoidratada	21111813	1
Caelo	Lactose monoidratada	220000736007	1
Caelo	Lactose monoidratada	22000736001	4
Caelo	Lactose monoidratada	22000736003	4
Caelo	Lactose monoidratada	22000736005	7
Caelo	Lactose monoidratada	22000736006	6
Caelo	Lactose monoidratada	22000736007	8
Caelo	Lactose monoidratada	22000736008	4
Caelo	Lactose monoidratada	22000736009	3
Caelo	Lactose monoidratada	22000736010	4
Caelo	Lactose monoidratada	22000736011	4
Caelo	Lactose monoidratada	22000736012	2
Caelo	Lactose monoidratada	22000736017	1
Caelo	Lactose monoidratada	220401LM	1
Caelo	Lactose monoidratada	23001015002	1
Caelo	Lactose monoidratada	23001015003	3
Caelo	Lactose monoidratada	23001015007	1
Caelo	Lactose monoidratada	23002236003	1
Caelo	Lactose monoidratada	23051501	1
Caelo	Lactose monoidratada	23061504	1
Caelo	Lactose monoidratada	23101404	1
Caelo	Lactose monoidratada	24011405	1
Caelo	Lactose monoidratada	26061801	1
Caelo	Lactose monoidratada	26071401	1
Caelo	Lactose monoidratada	27101702	1
Caelo	Lactose monoidratada	2901312210	1
Caelo	Lactose monoidratada	30031503	1
Caelo	Lactose monoidratada	30081801	1
Caelo	Lactose monoidratada	30101201	1
Caelo	Lactose monoidratada	3031501	1
Caelo	Lactose monoidratada	3091405	1
Caelo	Lactose monoidratada	3121406	1
Caelo	Lactose monoidratada	3295	1
Caelo	Lactose monoidratada	3788916	1
Caelo	Lactose monoidratada	4313Q2210	1
Caelo	Lactose monoidratada	5011901	1
Caelo	Lactose monoidratada	5041702	1
Caelo	Lactose monoidratada	5061504	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monoidratada	6091301	1
Caelo	Lactose monoidratada	6101702	1
Caelo	Lactose monoidratada	7031402	1
Caelo	Lactose monoidratada	7111402	1
Caelo	Lactose monoidratada	8021401	1
Caelo	Lactose monoidratada	8071501	1
Caelo	Lactose monoidratada	9051401	1
Caelo	Lactose monoidratada	9061803	1
Caelo	Lactose monoidratada	C1023	1
Caelo	Lactose monoidratada	s-100513-1	1
Caelo	Lactose monoidratada	Testmessung	1
Caeo/Noweda	Lactose monoidratada	1523204	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198023	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198002	2
Caesar & Loretz GmbH...	Lactose monoidratada	18198008	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198014	2
Caesar & Loretz GmbH...	Lactose monoidratada	18198017	1
Caesar & Loretz GmbH...	Lactose monoidratada	19137601	3
Caesar & Loretz GmbH...	Lactose monoidratada	192364003	3
Caesar & Loretz GmbH...	Lactose monoidratada	192364012	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198006	1
Caesar & Loretz GmbH...	Lactose monoidratada	192364008	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198016	1
Caesar & Loretz GmbH/AHD	Lactose monoidratada	22000736007	1
Caesar & Loretz GmbH...	Lactose monoidratada	192364016	2
Caesar & Loretz GmbH...	Lactose monoidratada	22000736015	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198023	1
Caesar & Loretz GmbH...	Lactose monoidratada	192364011	2
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	18198002	2
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	19137601	3
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	192364002	1
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	192364003	2
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	192364014	2
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	20004200001	1
Caesar & Loretz GmbH/Gehe	Lactose monoidratada	20004200005	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198014	1
Caesar & Loretz GmbH...	Lactose monoidratada	20004200001	1
Caesar & Loretz GmbH...	Lactose monoidratada	20004200005	1
Caesar & Loretz GmbH...	Lactose monoidratada	20004200009	1
Caesar & Loretz GmbH...	Lactose monoidratada	21001507005	1
Caesar & Loretz GmbH...	Lactose monoidratada	22000736001	1
Caesar & Loretz GmbH...	Lactose monoidratada	22000736009	2
Caesar & Loretz GmbH...	Lactose monoidratada	22000736018	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198007	1
Caesar & Loretz GmbH/Kehr	Lactose monoidratada	192364012	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198022	3
Caesar & Loretz GmbH...	Lactose monoidratada	192364016	3
Caesar & Loretz GmbH/L10	Lactose monoidratada	192364009	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198007	1
Caesar & Loretz GmbH...	Lactose monoidratada	21001507004	1
Caesar & Loretz GmbH...	Lactose monoidratada	22000736008	1
Caesar & Loretz GmbH...	Lactose monoidratada	18198017	2
Caesar & Loretz GmbH...	Lactose monoidratada	192364002	1
Caesar & Loretz GmbH...	Lactose monoidratada	19137601	2
Caesar & Loretz GmbH...	Lactose monoidratada	192364016	1
Caesar & Loretz GmbH...	Lactose monoidratada	20004200007	1
Caesar & Loretz GmbH...	Lactose monoidratada	20004200009	1
Caesar & Loretz GmbH	Lactose monoidratada	14140311	1
Caesar & Loretz GmbH	Lactose monoidratada	17321001	1
Caesar & Loretz GmbH	Lactose monoidratada	17336002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Lactose monoidratada	17336007	3
Caesar & Loretz GmbH	Lactose monoidratada	17336009	1
Caesar & Loretz GmbH	Lactose monoidratada	17336013	3
Caesar & Loretz GmbH	Lactose monoidratada	18198001	7
Caesar & Loretz GmbH	Lactose monoidratada	18198002	11
Caesar & Loretz GmbH	Lactose monoidratada	18198003	3
Caesar & Loretz GmbH	Lactose monoidratada	18198006	4
Caesar & Loretz GmbH	Lactose monoidratada	18198007	6
Caesar & Loretz GmbH	Lactose monoidratada	18198008	3
Caesar & Loretz GmbH	Lactose monoidratada	18198013	2
Caesar & Loretz GmbH	Lactose monoidratada	18198014	5
Caesar & Loretz GmbH	Lactose monoidratada	18198016	7
Caesar & Loretz GmbH	Lactose monoidratada	18198018	1
Caesar & Loretz GmbH	Lactose monoidratada	18198023	4
Caesar & Loretz GmbH	Lactose monoidratada	19137601	3
Caesar & Loretz GmbH	Lactose monoidratada	192364001	1
Caesar & Loretz GmbH	Lactose monoidratada	192364002	6
Caesar & Loretz GmbH	Lactose monoidratada	192364003	2
Caesar & Loretz GmbH	Lactose monoidratada	192364008	2
Caesar & Loretz GmbH	Lactose monoidratada	192364009	4
Caesar & Loretz GmbH	Lactose monoidratada	192364011	10
Caesar & Loretz GmbH	Lactose monoidratada	192364012	8
Caesar & Loretz GmbH	Lactose monoidratada	192364014	10
Caesar & Loretz GmbH	Lactose monoidratada	192364015	7
Caesar & Loretz GmbH	Lactose monoidratada	192364016	1
Caesar & Loretz GmbH	Lactose monoidratada	19236403	3
Caesar & Loretz GmbH	Lactose monoidratada	20004200001	2
Caesar & Loretz GmbH	Lactose monoidratada	20004200004	8
Caesar & Loretz GmbH	Lactose monoidratada	20004200005	2
Caesar & Loretz GmbH	Lactose monoidratada	20004200006	2
Caesar & Loretz GmbH	Lactose monoidratada	20004200007	3
Caesar & Loretz GmbH	Lactose monoidratada	20004200009	2
Caesar & Loretz GmbH	Lactose monoidratada	21001507003	12
Caesar & Loretz GmbH	Lactose monoidratada	21001507004	1
Caesar & Loretz GmbH	Lactose monoidratada	21001507005	1
Caesar & Loretz GmbH	Lactose monoidratada	22000736001	7
Caesar & Loretz GmbH	Lactose monoidratada	22000736003	1
Caesar & Loretz GmbH	Lactose monoidratada	22000736005	6
Caesar & Loretz GmbH	Lactose monoidratada	22000736006	1
Caesar & Loretz GmbH	Lactose monoidratada	22000736007	1
Caesar & Loretz GmbH	Lactose monoidratada	22000736008	3
Caesar & Loretz GmbH	Lactose monoidratada	22000736009	1
Caesar & Loretz GmbH	Lactose monoidratada	22000736015	1
Caesar & Loretz GmbH	Lactose monoidratada	22000736016	2
Caesar & Loretz GmbH	Lactose monoidratada	22000736018	2
Caesar & Loretz GmbH	Lactose monoidratada	23001015001	1
Caesar & Loretz GmbH	Lactose monoidratada	23001015003	1
Caesar & Loretz Hilden	Lactose monoidratada	18198013	1
Caesar & Loretz Hilden	Lactose monoidratada	192364015	1
Caesar & Loretz Hilden	Lactose monoidratada	19236403	1
Caesar & Loretz/Geil...	Lactose monoidratada	18198006	1
Caesar & Loretz/Geil...	Lactose monoidratada	18198018	1
Caesar & Loretz/Geil...	Lactose monoidratada	192364009	1
Caesar & Loretz/Geil...	Lactose monoidratada	192364015	2
Caesar & Loretz/Noweda	Lactose monoidratada	15236204	1
Caesar & Loretz/Noweda	Lactose monoidratada	17336013	1
Caesar /phönix	Lactose monoidratada	13104901	2
Caesar Loretz	Lactose monoidratada	21001507004	1
Caesar u Loretz	Lactose monoidratada	1433520	1
Caesar u Loretz	Lactose monoidratada	16231202	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar u. Loretz	Lactose monoidratada	14025620	1
Caesar& Loretz GmbH	Lactose monoidratada	22000736005	1
Cealo	Lactose monoidratada	13104901	1
Cealo	Lactose monoidratada	16231202	1
cealo	Lactose monoidratada	1733002	1
cealo	Lactose monoidratada	21001507003	1
Celo/Kehr	Lactose monoidratada	16231213	2
cesar&lorentz/Phönix	Lactose monoidratada	12336815	1
Chiesi	Lactose monoidratada	16027708	1
Dr.Wolff/Noweda	Lactose monoidratada	14A30-B07-296182	1
Ebert u. Jacobi 1...	Lactose monoidratada	15236215	1
Edelweiss/Fiebig	Lactose monoidratada	279325290-0555	1
Edelweiss/Fiebig	Lactose monoidratada	293272062-0535	1
Edelweiss/Fiebig	Lactose monoidratada	294237160-1115	1
Edelweiss/Geibo	Lactose monoidratada	258710315-1203	1
Edelweiss	Lactose monoidratada	253292176-1124	1
Edelweiss	Lactose monoidratada	283256067-0930	1
Edelweiss	Lactose monoidratada	6886	1
Eigen	Lactose monoidratada	129I20	1
Eigen	Lactose monoidratada	129I21	1
Eigenherstellung/ De...	Lactose monoidratada	10112101	1
Eigenherstellung	Lactose monoidratada	110913HJK01	1
Eigenherstellung	Lactose monoidratada	40113HJK01	1
Eigenherstellung	Lactose monoidratada	40815HMS01	1
Eigenherstellung	Lactose monoidratada	60814HSA01	1
Eigenherstellung	Lactose monoidratada	70113HML01	1
EuRho	Lactose monoidratada	1112020-01	1
EuRho	Lactose monoidratada	1112020-02	2
EuRho	Lactose monoidratada	1301028-01	1
EuRho	Lactose monoidratada	1501017-01	1
EuRho	Lactose monoidratada	1509030-02	1
EuRho	Lactose monoidratada	1606025-02	1
EuRho	Lactose monoidratada	170301901	3
Eurho	Lactose monoidratada	1802002-01	2
EuRho	Lactose monoidratada	1909014-01	2
Euro OCT	Lactose monoidratada	1401003-01	3
Euro OTC	Lactose monoidratada	1013Q-02210	1
Euro OTC	Lactose monoidratada	110602202	1
Euro OTC	Lactose monoidratada	1112020-01	2
Euro OTC	Lactose monoidratada	1112020-02	4
Euro OTC	Lactose monoidratada	130102801	1
Euro OTC	Lactose monoidratada	1301028-01	8
Euro OTC	Lactose monoidratada	1301028-02	12
Euro OTC	Lactose monoidratada	1301028-03	2
Euro OTC	Lactose monoidratada	1401003	1
Euro OTC	Lactose monoidratada	1401003-01	10
Euro OTC	Lactose monoidratada	140-1003-01	1
Euro OTC	Lactose monoidratada	140100302	1
Euro OTC	Lactose monoidratada	1401003-02	7
Euro OTC	Lactose monoidratada	14025604	2
Euro OTC	Lactose monoidratada	14025616	2
Euro OTC	Lactose monoidratada	15010	1
Euro OTC	Lactose monoidratada	150101701	1
Euro OTC	Lactose monoidratada	1501017-01	11
Euro OTC	Lactose monoidratada	1501017-02	1
Euro OTC	Lactose monoidratada	1509030-01	7
Euro OTC	Lactose monoidratada	150903002	1
Euro OTC	Lactose monoidratada	1509030-02	7
Euro OTC	Lactose monoidratada	15090-30-02	1
Euro OTC	Lactose monoidratada	160602501	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Lactose monoidratada	1606025-01	30
Euro OTC	Lactose monoidratada	1606025-02	4
Euro OTC	Lactose monoidratada	1703019-01	6
Euro OTC	Lactose monoidratada	1703019-02	6
Euro OTC	Lactose monoidratada	17A11-B01-334251	1
Euro OTC	Lactose monoidratada	180200201	2
Euro OTC	Lactose monoidratada	1802002-01	12
Euro OTC	Lactose monoidratada	1802002-02	1
Euro OTC	Lactose monoidratada	1802002-03	1
Euro OTC	Lactose monoidratada	180202-01	1
Euro OTC	Lactose monoidratada	18082014A	1
Euro OTC	Lactose monoidratada	1812008-01	14
Euro OTC	Lactose monoidratada	1812008-02	8
Euro OTC	Lactose monoidratada	1812008-03	2
Euro OTC	Lactose monoidratada	1909014-01	23
Euro OTC	Lactose monoidratada	1909014-02	2
Euro OTC	Lactose monoidratada	2005026	1
Euro OTC	Lactose monoidratada	200502601	2
Euro OTC	Lactose monoidratada	2005026-01	12
Euro OTC	Lactose monoidratada	2005026-0108597888	1
Euro OTC	Lactose monoidratada	2005026-02	2
Euro OTC	Lactose monoidratada	20052026-02	1
Euro OTC	Lactose monoidratada	2201013-01	5
Euro OTC	Lactose monoidratada	2208008-01	3
Euro OTC	Lactose monoidratada	31102013A	1
Euro OTC	Lactose monoidratada	3215A-02210	1
Euro OTC	Lactose monoidratada	5123	1
Euro OTC	Lactose monoidratada	L101852618	1
Euro OTC	Lactose monoidratada	L101854417A545	1
Euro OTC	Lactose monoidratada	L1237A4172	2
Euro OTC	Lactose monoidratada	UP250171017	1
Euro/Phönix	Lactose monoidratada	1802002-01	1
Euro/Phönix	Lactose monoidratada	1909014-01	2
Euroo/Phoenix	Lactose monoidratada	1401003-02	1
Europ Ots Pharma	Lactose monoidratada	1301028-02	3
Europ Ots Pharma	Lactose monoidratada	1401003-02	1
Europharm/Otto	Lactose monoidratada	1106022-01	1
Fagron	Lactose monoidratada	10726158	1
Fagron	Lactose monoidratada	10751120	1
Fagron	Lactose monoidratada	11C29-N06	1
Fagron	Lactose monoidratada	11L22-N03	1
Fagron	Lactose monoidratada	12/23-B02-287554	1
Fagron	Lactose monoidratada	12C09-N04	1
Fagron	Lactose monoidratada	12C26-N05	1
Fagron	Lactose monoidratada	12G27-N02	5
Fagron	Lactose monoidratada	13/23-B02-287554	1
Fagron	Lactose monoidratada	1301C005-278129	2
Fagron	Lactose monoidratada	1301C006-278128	6
Fagron	Lactose monoidratada	1301C007-278131	1
Fagron	Lactose monoidratada	1303C001	1
Fagron	Lactose monoidratada	1303C001-280388	1
Fagron	Lactose monoidratada	1303C002-280398	1
Fagron	Lactose monoidratada	1303C003	1
Fagron	Lactose monoidratada	1303C003-280390	1
Fagron	Lactose monoidratada	13E23-B01	2
Fagron	Lactose monoidratada	13E23-B01-283332	2
Fagron	Lactose monoidratada	13E23-B01-283334	1
Fagron	Lactose monoidratada	13I23-B03	4
Fagron	Lactose monoidratada	13I23-B03-287414	1
Fagron	Lactose monoidratada	13I23-B03-291115	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lactose monoidratada	13I23-B03-291116	1
Fagron	Lactose monoidratada	13J23-B03-291114	1
Fagron	Lactose monoidratada	14140312	1
Fagron	Lactose monoidratada	14333518	1
Fagron	Lactose monoidratada	14333525	1
Fagron	Lactose monoidratada	14A30-B07	2
Fagron	Lactose monoidratada	14A30-B07-296182	2
Fagron	Lactose monoidratada	14H27-B01-305666	1
Fagron	Lactose monoidratada	14H27-B02	1
Fagron	Lactose monoidratada	14H27-B02-302033	2
Fagron	Lactose monoidratada	15A19-B06	4
Fagron	Lactose monoidratada	15A19-B06-303437	3
Fagron	Lactose monoidratada	15A19-B06-303439	8
Fagron	Lactose monoidratada	15H14-B03-314451	3
Fagron	Lactose monoidratada	16231215	1
Fagron	Lactose monoidratada	1623123	1
Fagron	Lactose monoidratada	16A05-B03	1
Fagron	Lactose monoidratada	17078302	1
Fagron	Lactose monoidratada	17321001	1
Fagron	Lactose monoidratada	17336007	2
Fagron	Lactose monoidratada	1802002-01	1
Fagron	Lactose monoidratada	18B15-B06-353917	1
Fagron	Lactose monoidratada	18B15-B06-35917	1
Fagron	Lactose monoidratada	2005026-02	2
Fagron	Lactose monoidratada	282567/0	1
Fiebig	Lactose monoidratada	19236403	2
Finteler Apotheke	Lactose monoidratada	16231211	1
Fragon	Lactose monoidratada	10706040	1
Gatt-Koller / Phoenix	Lactose monoidratada	5580/12120813	2
Gatt-Koller	Lactose monoidratada	1702456	1
GEHE am 17.06.2014	Lactose monoidratada	13299108	1
Gehe/Caesar & Loretz GmbH	Lactose monoidratada	18198002	3
Gehe	Lactose monoidratada	1112020-01	1
Gehe	Lactose monoidratada	1112020-02	3
Gehe	Lactose monoidratada	1301028-02	2
Gehe	Lactose monoidratada	14025620	1
Gehe	Lactose monoidratada	14333502	1
gehe	Lactose monoidratada	16231211	1
Gehe	Lactose monoidratada	16231211	1
Gehe	Lactose monoidratada	17078303	2
GEHE	Lactose monoidratada	17321001	1
GEHE	Lactose monoidratada	17321006	2
GEHE	Lactose monoidratada	17336005	1
GEHE	Lactose monoidratada	17336008	1
GEHE	Lactose monoidratada	17336014	2
Gehe	Lactose monoidratada	1802002-01	1
Gehe	Lactose monoidratada	18198001	1
GEHE	Lactose monoidratada	18198008	2
Gehe	Lactose monoidratada	18198014	1
GEHE	Lactose monoidratada	18198017	1
Gehe	Lactose monoidratada	2300101004	1
Gehe	Lactose monoidratada	23001015004	2
Geilenkirchen	Lactose monoidratada	17336014	1
Geilenkirchen	Lactose monoidratada	18198002	3
Geilenkirchen	Lactose monoidratada	192364003	2
Geilenkirchen	Lactose monoidratada	192364016	4
Geilenkirchen	Lactose monoidratada	21001507005	2
Geilenkirchen	Lactose monoidratada	22000736006	1
Jenne	Lactose monoidratada	192364002	1
Jenne	Lactose monoidratada	23002236003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr 15.09.2020	Lactose monoidratada	192364011	1
Kehr	Lactose monoidratada	17321004	1
Kehr	Lactose monoidratada	22000736008	1
Kehr	Lactose monoidratada	22000736018	1
Kehr	Lactose monoidratada	23001015007	1
kölln GmbH	Lactose monoidratada	305749041-1056	1
Kölln GmbH	Lactose monoidratada	316349	1
L10	Lactose monoidratada	1606025-01	1
L12	Lactose monoidratada	1703019-01	1
L30	Lactose monoidratada	1703019-02	1
L30	Lactose monoidratada	1802002-01	1
Maros/Phoenix	Lactose monoidratada	192364012	1
Max Jenne	Lactose monoidratada	23003217001	1
Nachprüfung	Lactose monoidratada	3712Q-02210	1
Noweda/ Caesar&Loretz	Lactose monoidratada	12336815	1
Noweda	Lactose monoidratada	14025601	1
Noweda	Lactose monoidratada	16231215	1
Noweda	Lactose monoidratada	1703019-01	1
Noweda	Lactose monoidratada	1703019-02	1
Noweda	Lactose monoidratada	17078303	1
Noweda	Lactose monoidratada	1802002-01	3
Noweda	Lactose monoidratada	1802002-02	1
Noweda	Lactose monoidratada	1812008-02	1
Noweda	Lactose monoidratada	1812008-03	1
Noweda	Lactose monoidratada	1909014-01	2
Noweda	Lactose monoidratada	192364014	1
Noweda	Lactose monoidratada	21001507003	1
Noweda	Lactose monoidratada	22000736011	3
Noweda	Lactose monoidratada	22000736015	1
Noweda	Lactose monoidratada	23001015001	1
Noweda	Lactose monoidratada	23001015007	1
Noweda	Lactose monoidratada	L101854417A545	1
Otto Fischar GmbH	Lactose monoidratada	16231202	1
Otto Geilenkirchen GmbH	Lactose monoidratada	18198007	2
otz pharma	Lactose monoidratada	130102802	1
Peter Kölln GmbH & C…	Lactose monoidratada	256549266-0636	1
Peter Kölln	Lactose monoidratada	229719241-0640	1
pharmachem	Lactose monoidratada	15236208	1
Phoenix 19.03.2014	Lactose monoidratada	13104909	1
Phoenix 19.1.2019	Lactose monoidratada	18198001	1
Phoenix 20.09.19	Lactose monoidratada	1802002-01	3
Phoenix 30.04.2014	Lactose monoidratada	13E23-B01-283332	1
Phoenix	Lactose monoidratada	1404PLV-1928	4
Phoenix	Lactose monoidratada	15A19-B06	3
Phoenix	Lactose monoidratada	17321001	1
Phoenix	Lactose monoidratada	17336013	1
Phoenix	Lactose monoidratada	1909014-01	1
Phoenix	Lactose monoidratada	23003217001	1
Phoenix	Lactose monoidratada	3194	1
Phönix 17.05.2019	Lactose monoidratada	1812008-01	3
Phönix 28.08.2019	Lactose monoidratada	1812008-02	2
Phönix	Lactose monoidratada	12336815	1
Phönix	Lactose monoidratada	13299102	2
Phönix	Lactose monoidratada	14025616	1
Phönix	Lactose monoidratada	16027701	1
phönix	Lactose monoidratada	16231202	1
PHÖNIX	Lactose monoidratada	16A05-B03-322529	2
Phönix	Lactose monoidratada	17321001	1
Phönix	Lactose monoidratada	181200801	1
Phönix	Lactose monoidratada	18198001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Lactose monoidratada	18198007	1
Phönix	Lactose monoidratada	192364012	1
phönix	Lactose monoidratada	22000736005	1
Rondell Apotheke	Lactose monoidratada	1509030-01	2
Sana/Hanse	Lactose monoidratada	23003217003	1
Sanacorp,05.04.17, 5,96EUR	Lactose monoidratada	16231202	1
Sanacorp	Lactose monoidratada	12336815	1
Sanacorp	Lactose monoidratada	13104901	1
Sanacorp	Lactose monoidratada	13104909	1
Sanacorp	Lactose monoidratada	13299102	1
Sanacorp	Lactose monoidratada	13299108	1
Sanacorp	Lactose monoidratada	14025620	1
Sanacorp	Lactose monoidratada	14333509	1
Sanacorp	Lactose monoidratada	14333518	1
Sanacorp	Lactose monoidratada	16231215	1
Sanacorp	Lactose monoidratada	17078303	1
Sanacorp	Lactose monoidratada	17078306	1
Sanacorp	Lactose monoidratada	17078312	1
Sanacorp	Lactose monoidratada	17321001	1
Sanacorp	Lactose monoidratada	17321004	1
Sanacorp	Lactose monoidratada	1802002	1
Sanacorp	Lactose monoidratada	18198016	1
Sanacorp	Lactose monoidratada	192364002	1
Sanacorp	Lactose monoidratada	22000736005	2
sanacorp	Lactose monoidratada	22000736008	1
Sanacorp	Lactose monoidratada	22000736017	1
Sanacorp	Lactose monoidratada	23001015004	1
Sanacorp	Lactose monoidratada	23001015007	1
Sanacorp	Lactose monoidratada	23002236003	1
Sanacorp	Lactose monoidratada	274600148-0724	1
Sanacorp	Lactose monoidratada	274600148-0726	1
Sanacorp	Lactose monoidratada	283259077-1133	2
Sanacorp	Lactose monoidratada	283259077-1214	1
Sanacorp	Lactose monoidratada	285739172-1842	2
Sanacorp	Lactose monoidratada	285739172-1852	2
Sanacorp	Lactose monoidratada	285739172-1853	1
schubert / Phoenix	Lactose monoidratada	1334PLV-1775	1
siehe Protokoll	Lactose monoidratada	1606025-01	1
Spangropharm	Lactose monoidratada	91444379	1
vdl	Lactose monoidratada	1112020-01	2
Zentralapotheke Wetzlar	Lactose monoidratada	213L20	1

- 233 602 spectra from 1515 *Apo-Ident* customers from a total of 48 750 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lactose monoidratada* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lactose monoidratada* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	430	0	152 532
Type B	0	620	0	201 464
Type C	0	2459	6	233 602

The substance/substance group *Lactose monoidratada* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6047 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.7566 % (> 99.6349 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20685	22460	5,62	65,73
21525	22460	6,99	63,19
21526	22460	8,27	62,10
21527	22460	6,64	62,48
21528	22460	7,24	63,06
21529	22460	5,46	64,97
21935	21935	0,00	71,20
22460	22460	0,00	69,98
22701	22701	0,00	69,40
24929	24929	0,00	72,48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**L-alanina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	23776-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

L-alanina; Alanina levógira; Alaninum; Levoalanina

Special notes

When selecting the *L-alanina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
L-alanina	3	1	1

Second-stage model

For differentiation of the substance/substance group *L-alanina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *L-alanina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	70,74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *L-alanina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *L-alanina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	L-alanina	1710009	23776	40	20171018*
Euro OTC	L-alanina	2008025	25396	40	20200910*
Fagron	L-alanina	23F28-B02-230972	26905	40	20230721

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *L-alanina*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 842 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *L-alanina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-alanina	1601033-01	23905	40
Fagron	L-alanina	23F28-B02-230972	26905SI†	20

- 202 024 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *L-alanina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	L-alanina	2008025-01	2

- 236 065 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *L-alanina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-alanina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	60	0	202 024
Type C	0	2	0	236 065

The substance/substance group *L-alanina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9013 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23776	23776	0,00	175,60
25396	25396	0,00	158,45
26905	25396	17,13	168,92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lecitina de soja (forma instantânea)**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20539-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lecitina de soja (forma instantânea); Lecithinum e sojae plv.

Special notes

When selecting the *Lecitina de soja (forma instantânea)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lecitina de soja (forma instantânea)	5	2	40

Second-stage model

For differentiation of the substance/substance group *Lecitina de soja (forma instantânea)* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lecitina de soja (forma instantânea)* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mupirocina cálcica	69,50	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lecitina de soja (forma instantânea)* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lecitina de soja (forma instantânea)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lecitina de soja (forma i…	13030504	20985	40	1404399
Caelo	Lecitina de soja (forma i…	13279813	21523	40	20130903
Caelo	Lecitina de soja (forma i…	17118101	23370	40	20170620
Caelo	Lecitina de soja (forma i…	17118101	23445	40	20170620
Caelo	Lecitina de soja (forma i…	191879	24749	40	20190712*
Caelo	Lecitina de soja (forma i…	20002522003	25521	40	20200924

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Lecitina de soja (forma*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

instantânea). These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 722 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 2 reference samples from the substance/substance group *Lecitina de soja (forma instantânea)*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lecitina de soja (forma i…	173224	24244	40
Caelo	Lecitina de soja (forma i…	21001068004	25784	50

- 201 994 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 83 spectra from 46 *Apo-Ident* customers from 44 batches from the substance/substance group *Lecitina de soja (forma instantânea)*.

- Among them are spectra of independent samples from 40 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lecitina de soja (forma i…	23000766003	1
Caelo	Lecitina de soja (forma i…		1
Caelo	Lecitina de soja (forma i…	11371504	1
Caelo	Lecitina de soja (forma i…	12139001	3
Caelo	Lecitina de soja (forma i…	12139011	3
Caelo	Lecitina de soja (forma i…	12139012	1
Caelo	Lecitina de soja (forma i…	13030503	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lecitina de soja (forma i...	13030506	1
Caelo	Lecitina de soja (forma i...	13279806	1
Caelo	Lecitina de soja (forma i...	13279814	1
Caelo	Lecitina de soja (forma i...	14196305	1
Caelo	Lecitina de soja (forma i...	14281605	1
Caelo	Lecitina de soja (forma i...	14281606	2
Caelo	Lecitina de soja (forma i...	14281618	4
Caelo	Lecitina de soja (forma i...	14281620	1
Caelo	Lecitina de soja (forma i...	15262701	4
Caelo	Lecitina de soja (forma i...	15262704	4
Caelo	Lecitina de soja (forma i...	1526704	1
Caelo	Lecitina de soja (forma i...	16223302	4
Caelo	Lecitina de soja (forma i...	17081501	2
Caelo	Lecitina de soja (forma i...	17118101	1
Caelo	Lecitina de soja (forma i...	17118102	1
Caelo	Lecitina de soja (forma i...	17118105	2
Caelo	Lecitina de soja (forma i...	17118108	1
Caelo	Lecitina de soja (forma i...	17322401	3
Caelo	Lecitina de soja (forma i...	17322402	1
Caelo	Lecitina de soja (forma i...	17322405	5
Caelo	Lecitina de soja (forma i...	18282701	3
Caelo	Lecitina de soja (forma i...	19009101	3
Caelo	Lecitina de soja (forma i...	19009113	1
Caelo	Lecitina de soja (forma i...	20000718005	1
Caelo	Lecitina de soja (forma i...	20002522003	2
Caelo	Lecitina de soja (forma i...	21001068003	1
Caelo	Lecitina de soja (forma i...	21002621003	1
Caesar & Loretz GmbH Gehe	Lecitina de soja (forma i...	21001068004	1
Caesar & Loretz GmbH...	Lecitina de soja (forma i...	12139013	1
Caesar & Loretz GmbH...	Lecitina de soja (forma i...	20000718001	1
Caesar & Loretz GmbH...	Lecitina de soja (forma i...	20000718005	1
Caesar & Loretz GmbH...	Lecitina de soja (forma i...	19009110	1
Caesar & Loretz GmbH...	Lecitina de soja (forma i...	19009107	1
Caesar & Loretz GmbH	Lecitina de soja (forma i...	14281603	1
Caesar & Loretz GmbH	Lecitina de soja (forma i...	19009103	2
Caesar & Loretz GmbH	Lecitina de soja (forma i...	19187901	2
Caesar &Loretz GmbH	Lecitina de soja (forma i...	13030503	1
Caesar &Loretz GmbH	Lecitina de soja (forma i...	13279813	1
Gehe	Lecitina de soja (forma i...	19187901	1
Gehe	Lecitina de soja (forma i...	21002621003	1
INTR/ Sana	Lecitina de soja (forma i...	16223302	1
Sanacorp	Lecitina de soja (forma i...	14196305	1
Sanacorp	Lecitina de soja (forma i...	17322405	1
siehe WE-Prüfprotokoll	Lecitina de soja (forma i...	31/14	1

- 235 984 spectra from 1515 *Apo-Ident* customers from a total of 49 216 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lecitina de soja (forma instantânea)* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lecitina de soja (forma instantânea)* and it was evaluated how many matches (positive) and rejections (negative) were

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	90	0	201 994
Type C	0	83	0	235 984

The substance/substance group *Lecitina de soja (forma instantânea)* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.7711 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20985	20985	0,00	124,60
21523	20985	49,21	126,57
23370	20985	31,45	126,46
23445	20985	36,48	127,30
24749	24749	0,00	124,08
25521	20985	68,27	128,19

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Leucina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20970-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Leucina; Leucinum

Special notes

When selecting the *Leucina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Leucina	6	7	5

Second-stage model

For differentiation of the substance/substance group *Leucina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Leucina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Isoleucina	54,20	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Leucina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Leucina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Leucina	1302013-01	21612	60	20130320
Euro OTC	Leucina	1601032	22380	40	20160308*
Euro OTC	Leucina	2004006	25165	40	20200507*
Euro OTC	Leucina	2011008	25467	40	20201204*
Fagron	Leucina	13J09-N03	20970	40	1402431
Fagron	Leucina	15D09-B06-322249	23199	40	20151030

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Leucina*. These samples

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 330 spectra of 10 reference samples from the substance/substance group *Leucina*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Leucina	1708010	23607	40
Euro OTC	Leucina	1901008	24473	40
Euro OTC	Leucina	2203014	26041	40
Euro OTC	Leucina	2302005	26646	40
Euro OTC	Leucina	2401011	27144	40
Euro OTC	Leucina	2404015	27292	40
Fagron	Leucina	23F15-B10-231014	26907	40
Euro OTC	Leucina	2203014	26041SI	10
Euro OTC	Leucina	2302005	26646SI	20
Fagron	Leucina	23F15-B10-231014	26907SI	20

- 201 754 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Leucina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Leucina	1312032-01	1
Euro OTC	Leucina	1708010-01	2
Euro OTC	Leucina	700113	1
Fagron	Leucina	20J15-B02-202893	1
Fargon	Leucina	8160410903	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Leucina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Leucina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	330	0	201 754
Type C	0	6	0	236 061

The substance/substance group *Leucina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1818 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20970	20970	0,00	105,92
21612	25165	17,94	110,61

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22380	22380	0,00	111,28
23199	25467	12,39	115,70
25165	25165	0,00	115,04
25467	25467	0,00	114,43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Levedura de selênio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20906-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Levedura de selênio; Selênio levedura

Special notes

When selecting the *Levedura de selênio* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Levedura de selênio	5	2	5

Second-stage model

For differentiation of the substance/substance group *Levedura de selênio* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Levedura de selênio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	31,31	25,15
Fosfato sódico de riboflavina hidratado	69,20	–
⋮	⋮	⋮
Sulfato de colistina	>50	20,97
Bacitracina	>50	26,14
Anfotericina B	>50	27,65
Nistatina	>50	37,22
Riboflavina	>50	47,43
Estradiol hemi-hidratado	>50	52,52
Glicerofosfato de cálcio	>50	53,68
Carmelose sódica	>50	61,49
Pantotenato de cálcio	>50	62,24
Cianocobalamina	>50	71,20
Vitamina E acetato pó 50%	>50	82,54
Gelatina, branca	>50	83,31
Estriol	>50	92,50
SyrSpend® SF Alka	>50	93,75
Triancinolona	>50	105,76
Metilcobalamina	>50	132,15
Tosilcloramida sódica	>50	136,53
Amido de arroz	>50	140,36
Bromidrato de hioscina	>50	143,68
SyrSpend® SF pH4 neo	>50	164,42
Amido de milho	>50	174,47
Goma arábica, dispersão seca	>50	194,84
Ácido oxálico	>50	228,71
Maltodextrina	>50	252,81
Amido de trigo	>50	256,85
SyrSpend® SF pH4	>50	260,47
Fécula de batata	>50	297,40
Frutose	>50	395,94

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Levedura de selênio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Levedura de selênio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Levedura de selênio	13347911	21377	40	1509355
Caelo	Levedura de selênio	17002202	23120	40	1707512
Caelo	Levedura de selênio	17002208	23446	40	20170126
Caelo	Levedura de selênio	173332	24038	40	20180207*
Caelo	Levedura de selênio	192450005	25522	40	2106135

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Levedura de selênio*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 762 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Levedura de selênio*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Levedura de selênio	20003859005	25979	40
Euro OTC	Levedura de selênio	L1401013-01	21102	40
Caelo	Levedura de selênio	20003859005	25979SI	10

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 994 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Levedura de selênio*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Levedura de selênio	13347906	1
Caelo	Levedura de selênio	13347911	1
Caelo	Levedura de selênio	15276208	1
Caesar & Loretz GmbH...	Levedura de selênio	11318111	1
Euro OTC	Levedura de selênio	L1910012-01	1
Euro OTC	Levedura de selênio	L1910012-1	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Levedura de selênio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Levedura de selênio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	90	0	201 994
Type C	0	5	1	236 060

The substance/substance group *Levedura de selênio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9020 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21377	21377	0,00	78,05
23120	23120	0,00	65,96
23446	23120	5,21	63,32
24038	24038	0,00	70,75
25522	25522	0,00	72,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Levocarnitina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20357-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Levocarnitina; Carnitina levógira; L-carnitina

Special notes

When selecting the *Levocarnitina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Levocarnitina	7	9	20

Second-stage model

For differentiation of the substance/substance group *Levocarnitina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Levocarnitina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cistina	89,95	–
⋮	⋮	⋮
Valina	>50	80,66
Cloridrato de oxibutinina	>50	138,67
Capsaicina	>50	181,45
Citrato de sódio	>50	192,32
Prednicarbato	>50	242,22
Acetato de ciproterona	>50	257,34
Piridoxal-5-fosfato	>50	276,98
Metoxisaleno	>50	313,92
Alfaestradiol	>50	441,44
Cloridrato de quinina di-hidratado	>50	458,90
Cloridrato de amitriptilina	>50	468,12
Tetracaína	>50	471,37
Acetato de noretisterona	>50	491,07
Cloridrato de ciprofloxacina	>50	542,57
Heparina sódica	>50	839,92
Triclosan	>50	1346,42
Amifampridina	>50	2252,13
Sacarose	>50	2278,79

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Levocarnitina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Levocarnitina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Levocarnitina	1210029-01	20809	40	20121130
Euro OTC	Levocarnitina	2007040-01	25606	40	20201215

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Levocarnitina	2104006	25681	40	20210423*
Fagron	Levocarnitina	12H10-N07	20818	40	20120830
Fagron	Levocarnitina	14A20-B11-290728	21790	60	AR-15-FG-016322-01
Fagron	Levocarnitina	14A20-B11-290728	21968	60	AR-16-FG-005969-01
Fagron	Levocarnitina	15L04-B05-319229	23194	40	AR-17-FG-012937-01
Fagron	Levocarnitina	16L06-B03-338285	23919	40	20161227

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Levocarnitina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 12 reference samples from the substance/substance group *Levocarnitina*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Levocarnitina	1303027-02	21648	60
Euro OTC	Levocarnitina	2203025	26087	40
Euro OTC	Levocarnitina	2301027	26532	40
Euro OTC	Levocarnitina	2406011	27344	40
Euro OTC	Levocarnitina	2410001	27456	40
Fagron	Levocarnitina	16F20-B01-326616	23402	40
Fagron	Levocarnitina	17K23-B01-345633	24009	40
Fagron	Levocarnitina	22B02-B10-220587	26164	40
Fagron	Levocarnitina	24A05-B04-235963	27169	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Levocarnitina	2203025	26087SI	20
Euro OTC	Levocarnitina	2301027	26532SI	20
Fagron	Levocarnitina	22B02-B10-220587	26164SI	20

- 201 644 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 12 *Apo-Ident* customers from 21 batches from the substance/substance group *Levocarnitina*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Levocarnitina	2301027-01	1
Denk	Levocarnitina	A04217	1
EuRho	Levocarnitina	2007040-01	1
Euro OTC	Levocarnitina	1303027	1
Euro OTC	Levocarnitina	1705006-01	1
Euro OTC	Levocarnitina	1808027-01	1
Euro OTC	Levocarnitina	200402401	1
Euro OTC	Levocarnitina	2007040-01	3
Euro OTC	Levocarnitina	2203025-01	1
Euro OTC	Levocarnitina	L1608038-01	2
Euro OTC	Levocarnitina	L1705006-01	1
Euro OTC	Levocarnitina	L1801028-02	1
Euro OTC	Levocarnitina	L180802701	1
Fagron	Levocarnitina	13111701	1
Fagron	Levocarnitina	13G19-N12	2
Fagron	Levocarnitina	17K23-B01-346658	1
Fagron	Levocarnitina	19K08-F04	7
Fagron	Levocarnitina	19K08F04367748	2
Fagron	Levocarnitina	20B21-F01-370194	1
Fagron	Levocarnitina	20B21-F04	6
Fagron	Levocarnitina	9041504	1
Fagron	Levocarnitina	LC191017	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Levocarnitina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

relevant spectra of the various substances were compared with *Levocarnitina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	440	0	201 644
Type C	0	38	0	236 029

The substance/substance group *Levocarnitina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.2105 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20809	21790	29,34	194,35
20818	23194	30,32	207,28
21790	21790	0,00	197,76
21968	21968	0,00	186,62
23194	23194	0,00	184,75
23919	25681	24,29	193,77
25606	23194	29,79	210,38
25681	25681	0,00	170,75

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Levotiroxina sódica**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21708-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Levotiroxina sódica; Levothyroxinum natrii

Special notes

When selecting the *Levotiroxina sódica* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Levotiroxina sódica	6	4	3

Second-stage model

For differentiation of the substance/substance group *Levotiroxina sódica* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Levotiroxina sódica* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Eosina amarela	74,85	33,58
⋮	⋮	⋮
Cloreto de dequalínio	>50	71,18
Tanino	>50	121,78
Cloridrato de oxitetraciclina	>50	166,70
Ácido acetilsalicílico	>50	477,75
Ditranol	>50	561,99
Salicilato de sódio	>50	635,67
Ácido benzoico	>50	920,19

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Levotiroxina sódica* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Levotiroxina sódica*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Levotiroxina sódica	14E28-B05-298322	21708	30	1506426
Fagron	Levotiroxina sódica	14E28-B05-298322	21708SI	47	1506426
Fagron	Levotiroxina sódica	14E28-B05-306102	21820	60	20140915
Fagron	Levotiroxina sódica	14E28-B05-306102	21820SI	53	20140915
Fagron	Levotiroxina sódica	18G27-B02-352032	24286	40	20180822
Fagron	Levotiroxina sódica	20D01-F05-370575	25438	40	2110083
Fagron	Levotiroxina sódica	20D01-F05-370575	25438SI	39	2110083
Fagron	Levotiroxina sódica	20J01-F07-374963	25740	40	20201112
Fagron	Levotiroxina sódica	20J01-F07-374963	26080	40	20201112
Fagron	Levotiroxina sódica	20J01-F07-374963	26080SI	40	20201112
Fagron	Levotiroxina sódica	22C02-B03-223067	26333	40	20220613
Fagron	Levotiroxina sódica	22C02-B03-223067	26333SI	37	20220613

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 506 spectra of 12 reference samples from the substance/substance group *Levotiroxina sódica*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 456 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 364 spectra of 10 reference samples from the substance/substance group *Levotiroxina sódica*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Levotiroxina sódica	16G25-B99-329080	23191	40
Fagron	Levotiroxina sódica	17J10-B05-348764	24176	40
Fagron	Levotiroxina sódica	21I10-B10-217006	26068	40
Fagron	Levotiroxina sódica	23D29-B02-227893	27066	40
Fagron	Levotiroxina sódica	16G25-B99-329080	23191SI	24
Fagron	Levotiroxina sódica	17J10-B05-348764	24176SI	30
Fagron	Levotiroxina sódica	18G27-B02-352032	24286SI†	32
Fagron	Levotiroxina sódica	20J01-F07-374963	25740SI†	40
Fagron	Levotiroxina sódica	21I10-B10-217006	26068SI	40
Fagron	Levotiroxina sódica	23D29-B02-227893	27066SI	38

- 201 720 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 22 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Levotiroxina sódica*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Levotiroxina sódica	17J10-B05-345570	1
Fagron	Levotiroxina sódica	16G25-B99-324827	17
Fagron	Levotiroxina sódica	20D01-F05-370575	2
Fagron	Levotiroxina sódica	20J01-F07-374963	1
Fagron	Levotiroxina sódica	21/10-B10-217006	1

- 236 045 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Levotiroxina sódica* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Levotiroxina sódica* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	506	0	152 456
Type B	0	364	0	201 720
Type C	0	22	0	236 045

The substance/substance group *Levotiroxina sódica* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8142 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3516 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 72.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21708	21708	0,00	67,11
21820	25438	37,98	78,20
24286	25438	15,24	82,52
25438	25438	0,00	89,05
25740	25438	5,49	85,98
26080	25438	7,64	88,12
26333	25438	8,68	82,41

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**L-fenilalanina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21661-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

L-fenilalanina; Fenilalanina levógira; Phenylalaninum

Special notes

When selecting the *L-fenilalanina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
L-fenilalanina	7	6	4

Second-stage model

For differentiation of the substance/substance group *L-fenilalanina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *L-fenilalanina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de anfetamina	91,46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *L-fenilalanina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *L-fenilalanina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	L-fenilalanina	14088304	21661	60	1501656
Euro OTC	L-fenilalanina	1212014-03	21681	60	20130111
Euro OTC	L-fenilalanina	1704003	23173	40	20170425*
Euro OTC	L-fenilalanina	2307036	26861	40	20230823*
Euro OTC	L-fenilalanina	2307036	26861SI	20	20230823*
Fagron	L-fenilalanina	17B13-B03-343288	23936	40	20170309
Fagron	L-fenilalanina	19J23-F10-366142	24951	40	20191127
Fagron	L-fenilalanina	23C07-B05-227911	26671	40	20230327
Fagron	L-fenilalanina	23C07-B05-227911	26671SI	20	20230327

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *L-fenilalanina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 7 reference samples from the substance/substance group *L-fenilalanina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-fenilalanina	1409013-02	23024	40
Euro OTC	L-fenilalanina	1808022	24198	40
Euro OTC	L-fenilalanina	1907032	24846	40
Euro OTC	L-fenilalanina	2006038	25306	40
Euro OTC	L-fenilalanina	2105010	25711	50
Euro OTC	L-fenilalanina	2306009	26871	40
Euro OTC	L-fenilalanina	2306009	26871SI	20

- 201 814 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *L-fenilalanina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	L-fenilalanina	1409013-02	12
Euro OTC	L-fenilalanina	1704003-02	1
Euro OTC	L-fenilalanina	200603801	1
Euro OTC	L-fenilalanina	2006038-01	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *L-fenilalanina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-fenilalanina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	270	0	201 814
Type C	0	15	0	236 052

The substance/substance group *L-fenilalanina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21661	21661	0,00	134,90
21681	21661	25,17	167,33
23173	23173	0,00	199,96

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23936	21661	6,39	135,06
24951	21661	9,09	132,75
26671	21661	7,95	128,95
26861	26861	0,00	152,55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lidocaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20942-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lidocaína; Lidocainum

Special notes

When selecting the *Lidocaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lidocaína	9	14	389

Second-stage model

For differentiation of the substance/substance group *Lidocaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lidocaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	126,55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lidocaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lidocaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lidocaína	13352411	21673	60	20131115
Caelo	Lidocaína	180444	24031	40	20180419*
Euro OTC	Lidocaína	1310023-01	21640	60	20131118
Euro OTC	Lidocaína	1612021	22984	40	20170206*
Euro OTC	Lidocaína	1911005	24928	40	20191129*
Euro OTC	Lidocaína	2101035	25533	40	20210304*
Euro OTC	Lidocaína	2304015	26654	40	20230510*
Euro OTC	Lidocaína	2304015	26654SI	20	20230510*
Fagron	Lidocaína	13H05-N05	20942	40	1401378
Fagron	Lidocaína	16F21-B06-327232	23019	40	20160728

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Lidocaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 600 spectra of 16 reference samples from the substance/substance group *Lidocaína*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lidocaína	162895	22768	40
Caelo	Lidocaína	171831	23632	40
Caelo	Lidocaína	190545	24530	40
Caelo	Lidocaína	22000398	26736	40
Caelo	Lidocaína	23002079	26964	40
Euro OTC	Lidocaína	1603027	22526	40
Euro OTC	Lidocaína	1801032	23960	40
Euro OTC	Lidocaína	1902003	24475	40
Euro OTC	Lidocaína	1905004	24610	40
Euro OTC	Lidocaína	1908005	24847	40
Euro OTC	Lidocaína	2006013	25244	40
Euro OTC	Lidocaína	2206002	26230	40
Euro OTC	Lidocaína	2310020	27075	40
Fagron	Lidocaína	22C15-B17-216737	26134	40
Euro OTC	Lidocaína	2206002	26230SI	20
Fagron	Lidocaína	22C15-B17-216737	26134SI	20

- 201 484 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1728 spectra from 697 *Apo-Ident* customers from 418 batches from the substance/substance group *Lidocaína*.

- Among them are spectra of independent samples from 389 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lidocaína	1908005-01	1
	Lidocaína	20003343016	4
	Lidocaína	20H13-F04-373497	1
	Lidocaína	20L11-F01-376356	1
	Lidocaína	22000398003	2
	Lidocaína	22000398004	1
	Lidocaína	22000398010	1
	Lidocaína	22000398011	9
	Lidocaína	22000398013	5
	Lidocaína	22000398015	2
	Lidocaína	22000398016	7
	Lidocaína	2206002-01	1
	Lidocaína	22C15-B17	1
	Lidocaína	22C15-B17-216737	4
	Lidocaína	22C15-B17-216738	2
	Lidocaína	22C15-B17-216739	5
	Lidocaína	22c15-b17-225236	1
	Lidocaína	22C15-B17-225236	2
	Lidocaína	23002079001	1
	Lidocaína	2304015-01	1
	Lidocaína	23D25-B10-230220	1
	Lidocaína	23D25-B10-230226	2
	Lidocaína	B10-2302201	2
	Lidocaína	B17-2137307	1
	Lidocaína	LDB/722005	2
AHD	Lidocaína	15332314	1
AHD	Lidocaína	19054506	1
AHD	Lidocaína	22C15B17-225236	1
Alliance Healthcare	Lidocaína	19F27-B01-363501	1
Alliance Healthcare	Lidocaína	19F27-B01-363506	1
Alliance Healthcare	Lidocaína	20L11-F01-376356	1
Alliance Healthcare	Lidocaína	22C15-B17-225236	1
Alliance	Lidocaína	15H27-B07-318310	1
Alliance	Lidocaína	22000398010	1
Alliance	Lidocaína	22C15-B17-216737	1
Allianz Healthcare	Lidocaína	8565960	1
Alte Apotheke	Lidocaína	16A28B06-321297	1
Anzag	Lidocaína	12E30-N10	1
Audor Pharma	Lidocaína	1911005-01	1
Cae	Lidocaína	20003343010	1
Caelo	Lidocaína	11K17-N03	1
Caelo	Lidocaína	12163802	2
Caelo	Lidocaína	12163803	3
Caelo	Lidocaína	12163804	2
Caelo	Lidocaína	12163810	1
Caelo	Lidocaína	12163811	4
Caelo	Lidocaína	12163813	5
Caelo	Lidocaína	122294405	1
Caelo	Lidocaína	12294405	2
Caelo	Lidocaína	12294408	2
Caelo	Lidocaína	12294412	10
Caelo	Lidocaína	12294413	1
Caelo	Lidocaína	133522408	1
Caelo	Lidocaína	133524	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaína	13352403	1
Caelo	Lidocaína	13352405	1
Caelo	Lidocaína	13352406	1
Caelo	Lidocaína	13352408	9
Caelo	Lidocaína	13352411	6
Caelo	Lidocaína	13352413	3
Caelo	Lidocaína	13352414	2
Caelo	Lidocaína	13352415	3
Caelo	Lidocaína	13J30-B02-292221	1
Caelo	Lidocaína	14299301	2
Caelo	Lidocaína	14299303	2
Caelo	Lidocaína	14299305	2
Caelo	Lidocaína	1512003	1
Caelo	Lidocaína	15212001	2
Caelo	Lidocaína	15212002	4
Caelo	Lidocaína	15212003	3
Caelo	Lidocaína	15332302	5
Caelo	Lidocaína	15332303	1
Caelo	Lidocaína	15332305	2
Caelo	Lidocaína	15332306	3
Caelo	Lidocaína	15332309	2
Caelo	Lidocaína	15332310	4
Caelo	Lidocaína	15332314	2
Caelo	Lidocaína	15A15-B01-304284	3
Caelo	Lidocaína	15D23-B08	1
Caelo	Lidocaína	15H27-B07-318310	1
Caelo	Lidocaína	15H-B07-318310	1
Caelo	Lidocaína	16087702	1
Caelo	Lidocaína	16087703	1
Caelo	Lidocaína	16087704	8
Caelo	Lidocaína	16087707	9
Caelo	Lidocaína	16087708	1
Caelo	Lidocaína	16087709	1
Caelo	Lidocaína	16087710	3
Caelo	Lidocaína	16087711	10
Caelo	Lidocaína	16087712	7
Caelo	Lidocaína	1608774	1
Caelo	Lidocaína	160877708	1
Caelo	Lidocaína	1612021-04	1
Caelo	Lidocaína	16289502	11
Caelo	Lidocaína	16289503	10
Caelo	Lidocaína	16289504	2
Caelo	Lidocaína	16289507	2
Caelo	Lidocaína	16289508	19
Caelo	Lidocaína	1629508	1
Caelo	Lidocaína	16A28-B06-320059	1
Caelo	Lidocaína	16F21-806-333787	1
Caelo	Lidocaína	16F21-B06-323670	1
Caelo	Lidocaína	16F21-B06-326631	1
Caelo	Lidocaína	16F21-B06-328421	3
Caelo	Lidocaína	1718308	1
Caelo	Lidocaína	17183102	3
Caelo	Lidocaína	17183103	8
Caelo	Lidocaína	17183105	1
Caelo	Lidocaína	17183106	1
Caelo	Lidocaína	17183108	8
Caelo	Lidocaína	17183109	9
Caelo	Lidocaína	17348502	6
Caelo	Lidocaína	17348503	15
Caelo	Lidocaína	17348503P-190516-5	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaína	1783109	2
Caelo	Lidocaína	17G03-B08	1
Caelo	Lidocaína	17G03B08338286	1
Caelo	Lidocaína	17G03-B08-341306	3
Caelo	Lidocaína	17G03B08341308	1
Caelo	Lidocaína	17K23-B04-343250	1
Caelo	Lidocaína	17K23-B04-347473	1
Caelo	Lidocaína	17K23-B04-347475	1
Caelo	Lidocaína	17K23-B04-350189	1
Caelo	Lidocaína	17K23-B04-350543	1
Caelo	Lidocaína	17K23-B04-353247	1
Caelo	Lidocaína	17K23-B04-353427	1
Caelo	Lidocaína	18041812	1
Caelo	Lidocaína	1804404	1
Caelo	Lidocaína	1804410	1
Caelo	Lidocaína	1804413	2
Caelo	Lidocaína	18044402	5
Caelo	Lidocaína	18044404	9
Caelo	Lidocaína	18044405	8
Caelo	Lidocaína	18044408	7
Caelo	Lidocaína	18044410	12
Caelo	Lidocaína	18044412	2
Caelo	Lidocaína	18044413	17
Caelo	Lidocaína	18044414	1
Caelo	Lidocaína	18044415	6
Caelo	Lidocaína	180444404	1
Caelo	Lidocaína	190545001	15
Caelo	Lidocaína	19054503	15
Caelo	Lidocaína	19054503P-190909-3	1
Caelo	Lidocaína	19054505	8
Caelo	Lidocaína	19054506	18
Caelo	Lidocaína	19054507	2
Caelo	Lidocaína	192758001	5
Caelo	Lidocaína	192758002	1
Caelo	Lidocaína	192758003	1
Caelo	Lidocaína	192758004	8
Caelo	Lidocaína	192758005	13
Caelo	Lidocaína	19278005	1
Caelo	Lidocaína	1954503	1
Caelo	Lidocaína	19f27-b01-363506	2
Caelo	Lidocaína	19F27-B01-363506	1
Caelo	Lidocaína	20003343001	2
Caelo	Lidocaína	20003343002	5
Caelo	Lidocaína	20003343004	13
Caelo	Lidocaína	20003343006	3
Caelo	Lidocaína	20003343007	3
Caelo	Lidocaína	20003343008	11
Caelo	Lidocaína	20003343010	9
Caelo	Lidocaína	20003343011	4
Caelo	Lidocaína	20003343012	2
Caelo	Lidocaína	20003343014	3
Caelo	Lidocaína	20003343015	13
Caelo	Lidocaína	20003343016	5
Caelo	Lidocaína	2000334304	1
Caelo	Lidocaína	2000409002	1
Caelo	Lidocaína	20004099001	23
Caelo	Lidocaína	20004099002	2
Caelo	Lidocaína	2000409901	1
Caelo	Lidocaína	2003343008	1
Caelo	Lidocaína	200409900100	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaína	2004099002	1
Caelo	Lidocaína	20C13-F04-369814	1
Caelo	Lidocaína	20H13-F04-3734909	1
Caelo	Lidocaína	22000398001	3
Caelo	Lidocaína	22000398003	2
Caelo	Lidocaína	22000398004	19
Caelo	Lidocaína	22000398010	2
Caelo	Lidocaína	22000398011	1
Caelo	Lidocaína	220600-01	1
Caelo	Lidocaína	5111201	1
Caelo	Lidocaína	8629595	1
Caelo	Lidocaína	9205916	2
Caelo	Lidocaína	9205919	1
Caelo	Lidocaína	LDB/733005	2
Caesar & Loretz GmbH...	Lidocaína	20003343015	2
Caesar & Loretz GmbH...	Lidocaína	18044405	1
Caesar & Loretz GmbH /E	Lidocaína	18044413	1
Caesar & Loretz GmbH...	Lidocaína	20003343015	2
Caesar & Loretz GmbH/ AHD	Lidocaína	20003343010	1
Caesar & Loretz GmbH...	Lidocaína	192758004	1
Caesar & Loretz GmbH...	Lidocaína	22000398010	1
Caesar & Loretz GmbH...	Lidocaína	20003343002	1
Caesar & Loretz GmbH/AHC	Lidocaína	20003343015	1
Caesar & Loretz GmbH...	Lidocaína	20004099001	1
Caesar & Loretz GmbH...	Lidocaína	19054505	1
Caesar & Loretz GmbH/Gehe	Lidocaína	20003343006	1
Caesar & Loretz GmbH/Gehe	Lidocaína	20003343011	2
Caesar & Loretz GmbH...	Lidocaína	192758005	1
Caesar & Loretz GmbH...	Lidocaína	20003343004	2
Caesar & Loretz GmbH...	Lidocaína	192758004	2
Caesar & Loretz GmbH...	Lidocaína	20003343002	3
Caesar & Loretz GmbH...	Lidocaína	18044410	1
Caesar & Loretz GmbH...	Lidocaína	192758005	1
Caesar & Loretz GmbH...	Lidocaína	20003343004	2
Caesar & Loretz GmbH...	Lidocaína	20003343008	1
Caesar & Loretz GmbH...	Lidocaína	20004099001	1
Caesar & Loretz GmbH...	Lidocaína	19054505	1
Caesar & Loretz GmbH	Lidocaína	12294412	1
Caesar & Loretz GmbH	Lidocaína	17K23_B04_355709	1
Caesar & Loretz GmbH	Lidocaína	18044408	1
Caesar & Loretz GmbH	Lidocaína	18044410	2
Caesar & Loretz GmbH	Lidocaína	18044414	2
Caesar & Loretz GmbH	Lidocaína	18044415	3
Caesar & Loretz GmbH	Lidocaína	190545001	5
Caesar & Loretz GmbH	Lidocaína	19054503	1
Caesar & Loretz GmbH	Lidocaína	19054505	1
Caesar & Loretz GmbH	Lidocaína	19054506	2
Caesar & Loretz GmbH	Lidocaína	19054507	1
Caesar & Loretz GmbH	Lidocaína	192758001	1
Caesar & Loretz GmbH	Lidocaína	192758003	1
Caesar & Loretz GmbH	Lidocaína	192758004	2
Caesar & Loretz GmbH	Lidocaína	20003343001	1
Caesar & Loretz GmbH	Lidocaína	20003343002	8
Caesar & Loretz GmbH	Lidocaína	20003343004	7
Caesar & Loretz GmbH	Lidocaína	20003343006	2
CAESAR & LORETZ GMBH	Lidocaína	20003343006	1
Caesar & Loretz GmbH	Lidocaína	20003343008	1
Caesar & Loretz GmbH	Lidocaína	20003343010	4
Caesar & Loretz GmbH	Lidocaína	20003343011	2
Caesar & Loretz GmbH	Lidocaína	20003343014	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Lidocaína	20003343015	5
Caesar & Loretz GmbH	Lidocaína	20003343016	2
Caesar & Loretz GmbH	Lidocaína	20004099001	9
Caesar & Loretz GmbH	Lidocaína	22000398004	4
Caesar & Loretz GmbH	Lidocaína	22C15-B17-216739	1
Caesar & Loretz GmbHGehe	Lidocaína	22000398016	1
Caesar & Loretz Hilden	Lidocaína	19054506	1
Caesar&Loretz GmbH	Lidocaína	16289502	1
Caesar&Loretz,Phönix...	Lidocaína	15332314	1
Cealo / Anzag	Lidocaína	211217(20003343008)	1
Cealo	Lidocaína	17348503	1
Ebert-Jacobi	Lidocaína	16289504	1
Eur Rho Gehe	Lidocaína	1908005-92	1
EuRho, Noweda	Lidocaína	2101035-03	1
Euro OTC	Lidocaína	10129901	1
Euro OTC	Lidocaína	1310023-02	3
Euro OTC	Lidocaína	1603027-01	2
Euro OTC	Lidocaína	1603027-02	1
Euro OTC	Lidocaína	1612021-01	5
Euro OTC	Lidocaína	161202102	2
Euro OTC	Lidocaína	1612021-02	6
Euro OTC	Lidocaína	1612021-03	4
Euro OTC	Lidocaína	1612021-04	6
Euro OTC	Lidocaína	17348503	1
Euro OTC	Lidocaína	17K23B04345215	1
Euro OTC	Lidocaína	17K23-B04-347473	1
Euro OTC	Lidocaína	190200301	1
Euro OTC	Lidocaína	1902003-01	4
Euro OTC	Lidocaína	1905004-01	1
Euro OTC	Lidocaína	190800501	1
Euro OTC	Lidocaína	1908005-01	18
Euro OTC	Lidocaína	1908005-02	9
Euro OTC	Lidocaína	1911005-01	3
Euro OTC	Lidocaína	2006013-01	7
Euro OTC	Lidocaína	2101035-01	8
Euro OTC	Lidocaína	210103502	1
Euro OTC	Lidocaína	2101035-02	7
Euro OTC	Lidocaína	2101035-03	5
Euro OTC	Lidocaína	2206002-01	1
Euro OTC	Lidocaína	2206002-02	3
Euro OTC	Lidocaína	LD/119024	1
Euro OTC	Lidocaína	LDB/116106	1
Euro OTC	Lidocaína	LDB/120025	1
Fagro/Gehe	Lidocaína	15a15b01304284	1
Fagron	Lidocaína		2
Fagron	Lidocaína	1014I-07006	1
Fagron	Lidocaína	1113M-03584	1
Fagron	Lidocaína	1116E-07006	1
Fagron	Lidocaína	118J23-B02-359239	1
Fagron	Lidocaína	11C09-N07	2
Fagron	Lidocaína	11D28-N12	1
Fagron	Lidocaína	11K17-N03	1
Fagron	Lidocaína	12/21-N06	3
Fagron	Lidocaína	12C08-N11	2
Fagron	Lidocaína	12E30-N10	8
Fagron	Lidocaína	12h16_n05	1
Fagron	Lidocaína	12h16-N05	1
Fagron	Lidocaína	12H16-n05	1
Fagron	Lidocaína	12H16-N05	5
Fagron	Lidocaína	12I21N06	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaína	12I21-N06	3
Fagron	Lidocaína	12K13-N01	1
Fagron	Lidocaína	1330-B02-287641	1
Fagron	Lidocaína	13B27-N04	8
Fagron	Lidocaína	13E28-B40-289433	1
Fagron	Lidocaína	13H05-N05	10
Fagron	Lidocaína	13H05-N050171/245	1
Fagron	Lidocaína	13J30-B02	6
Fagron	Lidocaína	13J30-b02-287639	1
Fagron	Lidocaína	13J30-B02-287640	1
Fagron	Lidocaína	13J30-B02-287641	6
Fagron	Lidocaína	13j30B02292219	1
Fagron	Lidocaína	13J30-B02-292219	2
Fagron	Lidocaína	13J30-B02-292220	2
Fagron	Lidocaína	13J30-B02-292221	5
Fagron	Lidocaína	14E13-B05	2
Fagron	Lidocaína	14E13-B05-295549	4
Fagron	Lidocaína	14E13-B05-295550	2
Fagron	Lidocaína	14E13-B05-295552	3
Fagron	Lidocaína	15332305	1
Fagron	Lidocaína	15A15-B01	1
Fagron	Lidocaína	15A15-B01-304282	5
Fagron	Lidocaína	15A15-B01-304283	2
Fagron	Lidocaína	15A15B01304284	1
Fagron	Lidocaína	15A15-B01-304284	10
Fagron	Lidocaína	15D23-B08	1
Fagron	Lidocaína	15D23-B08_309882	1
Fagron	Lidocaína	15D23-B08_312058	1
Fagron	Lidocaína	15d23-b08-309882	1
Fagron	Lidocaína	15D23-B08-309882	1
Fagron	Lidocaína	15D23-B08-31058	1
Fagron	Lidocaína	15D23B08311708	1
Fagron	Lidocaína	15D23-B08-311708	1
Fagron	Lidocaína	15d23-b08-312058	2
Fagron	Lidocaína	15D23-B08-312058	11
Fagron	Lidocaína	15h27-b05-318310	1
Fagron	Lidocaína	15H27-B07	1
Fagron	Lidocaína	15H27-B07-315483	2
Fagron	Lidocaína	15H27-B07-316784	2
Fagron	Lidocaína	15H27-B07-318310	5
Fagron	Lidocaína	1612021-01	1
Fagron	Lidocaína	16289508	1
Fagron	Lidocaína	16A28B06320059	1
Fagron	Lidocaína	16A28-B06-320059	2
Fagron	Lidocaína	16A28-B06320079	1
Fagron	Lidocaína	16A28-B06-320079	1
Fagron	Lidocaína	16F21	2
Fagron	Lidocaína	16F21-B06	7
Fagron	Lidocaína	16F21-B06-323669	5
Fagron	Lidocaína	16F21-B06-323670	18
Fagron	Lidocaína	16F21B06325934	1
Fagron	Lidocaína	16F21-B06-325934	3
Fagron	Lidocaína	16F21-B06-327232	3
Fagron	Lidocaína	16F21-B06-328421	8
Fagron	Lidocaína	16F21-B06-328421	1
Fagron	Lidocaína	16F21-B06-329589	1
Fagron	Lidocaína	16F21B06332251	1
Fagron	Lidocaína	16F21-B06-332253	6
Fagron	Lidocaína	16F21-B06-332253	1
Fagron	Lidocaína	16F21B06333787	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaína	16F21-B06-333787	1
Fagron	Lidocaína	16F21-B06-333788	1
Fagron	Lidocaína	16f21-b06-335659	1
Fagron	Lidocaína	16F21-B06-335659	1
Fagron	Lidocaína	17G03-B08	5
Fagron	Lidocaína	17G03-B08-337576	2
Fagron	Lidocaína	17G03-B08-338284	1
Fagron	Lidocaína	17g03-b08-338286	1
Fagron	Lidocaína	17G03-B08-338286	6
Fagron	Lidocaína	17G03-B08-339445	2
Fagron	Lidocaína	17G03-B08-341306	5
Fagron	Lidocaína	17G03-B08-341308	5
Fagron	Lidocaína	17G03-B08-343251	4
Fagron	Lidocaína	17G23-B04-350541	1
Fagron	Lidocaína	17K23-B04	16
Fagron	Lidocaína	17K23-B04-343250	6
Fagron	Lidocaína	17K23-B04-345215	10
Fagron	Lidocaína	17K23-B04-345948	3
Fagron	Lidocaína	17K23B04347473	2
Fagron	Lidocaína	17K23-B04-347473	7
Fagron	Lidocaína	17K23B04347474	1
Fagron	Lidocaína	17K23-B04-347474	4
Fagron	Lidocaína	17k23-b04-347475	1
Fagron	Lidocaína	17K23-B04-347475	9
Fagron	Lidocaína	17k23-b04-349366	1
Fagron	Lidocaína	17K23B04350189	1
Fagron	Lidocaína	17K23-B04-350189	5
Fagron	Lidocaína	17K23-B04-350541	8
Fagron	Lidocaína	17K23-B04-350542	2
Fagron	Lidocaína	17K23-B04-350543	13
Fagron	Lidocaína	17K23-B04-353247	7
Fagron	Lidocaína	17k23-b04-353427	1
Fagron	Lidocaína	17K23-B04-353427	7
Fagron	Lidocaína	17K23-B04-3534274	1
Fagron	Lidocaína	17K23B04353428	1
Fagron	Lidocaína	17K23-B04-353428	7
Fagron	Lidocaína	17K23-B04-355709	13
Fagron	Lidocaína	17K23-B04-355750	1
Fagron	Lidocaína	18/23-B02-359237	1
Fagron	Lidocaína	18/23-B02-359239	1
Fagron	Lidocaína	1823-B02-356573	1
Fagron	Lidocaína	18J23-B02	8
Fagron	Lidocaína	18J23-B02_359237	1
Fagron	Lidocaína	18J23-B02-3557018	1
Fagron	Lidocaína	18J23-B02-355708	4
Fagron	Lidocaína	18J23-B02356573	1
Fagron	Lidocaína	18J-23-B02-356573	1
Fagron	Lidocaína	18J23-B02-35673	1
Fagron	Lidocaína	18j23-B02-359237	1
Fagron	Lidocaína	18J23-B02-359237	5
Fagron	Lidocaína	18J23-B02-359238	3
Fagron	Lidocaína	18J23B02359239	1
Fagron	Lidocaína	18J23-B02-359239	22
Fagron	Lidocaína	18j23bo2359239	1
Fagron	Lidocaína	190545001	1
Fagron	Lidocaína	190981109	1
Fagron	Lidocaína	19F27-B01	18
Fagron	Lidocaína	19F27-B01363500	1
Fagron	Lidocaína	19F27-B01-363500	7
Fagron	Lidocaína	19F27-B01-3635005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaína	19F27-B01-3635006	1
Fagron	Lidocaína	19f27-B01-363501	1
Fagron	Lidocaína	19F27-B01-363501	21
Fagron	Lidocaína	19F27-B01-363502	12
Fagron	Lidocaína	19f27b01363504	1
Fagron	Lidocaína	19F27-b01-363504	1
Fagron	Lidocaína	19F27-B01363504	1
Fagron	Lidocaína	19F27-B01-363504	10
Fagron	Lidocaína	19F27-B01-363505	8
Fagron	Lidocaína	19F27-B01-363506	15
Fagron	Lidocaína	19F27-B01-363511	1
Fagron	Lidocaína	19F27-Bo1-363504	2
Fagron	Lidocaína	19F27-BO1-363506	2
Fagron	Lidocaína	20C13-F04	4
Fagron	Lidocaína	20C13-F04-3698105	1
Fagron	Lidocaína	20C13-F04-3698106	1
Fagron	Lidocaína	20C13-F04-369814	4
Fagron	Lidocaína	20c13-F04-369815	1
Fagron	Lidocaína	20C13-F04-369815	9
Fagron	Lidocaína	20C13-F04-369816	13
Fagron	Lidocaína	20H13-F03	4
Fagron	Lidocaína	20H13-F03-373500	1
Fagron	Lidocaína	20H13-F03-373501	1
Fagron	Lidocaína	20H13-F04	4
Fagron	Lidocaína	20H13-F04-3734907	1
Fagron	Lidocaína	20H13-f04-373497	1
Fagron	Lidocaína	20H13-F04-373497	16
Fagron	Lidocaína	20H13-F04-373499	3
Fagron	Lidocaína	20H13-F04-373501	1
Fagron	Lidocaína	20h13-f04-73497	1
Fagron	Lidocaína	20H13-FO-373497	1
Fagron	Lidocaína	20H13FO4-373497	1
Fagron	Lidocaína	20ht3-f04-373497	1
Fagron	Lidocaína	20L11-F01	4
Fagron	Lidocaína	20L11-F01_376357	1
Fagron	Lidocaína	20L11-F01-376356	2
Fagron	Lidocaína	20l11-f01-376357	1
Fagron	Lidocaína	20L11-f01-376357	1
Fagron	Lidocaína	20L11-F01-376357	9
Fagron	Lidocaína	20M13-F04-373497	1
Fagron	Lidocaína	214U-03584	1
Fagron	Lidocaína	21B10-B07	1
Fagron	Lidocaína	21B10-B07-213330	3
Fagron	Lidocaína	21B10-B07-213578	1
Fagron	Lidocaína	21f08b14216888	1
Fagron	Lidocaína	22C115-B17-216739	1
Fagron	Lidocaína	22C15-817-216739	1
Fagron	Lidocaína	22C15-B17	2
Fagron	Lidocaína	22C15-B17_216737	1
Fagron	Lidocaína	22C15-B17-216737	9
Fagron	Lidocaína	22C15-B17-216738	10
Fagron	Lidocaína	22c15b17216739	1
Fagron	Lidocaína	22c15-b17-216739	1
Fagron	Lidocaína	22C15-B17-216739	20
Fagron	Lidocaína	22C15-B17-221066	1
Fagron	Lidocaína	22C15-B17-225236	1
Fagron	Lidocaína	22C15-B17-225237	1
Fagron	Lidocaína	20L11-FO1-376357	1
Fagron	Lidocaína	369816	1
Fagron	Lidocaína	5122014A	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaína	515M-07006	1
Fagron	Lidocaína	5742	1
Fagron	Lidocaína	6J23-No2	1
Fagron	Lidocaína	700412-0002	1
Fagron	Lidocaína	700412-0004	1
Fagron	Lidocaína	700412-0006	1
Fagron	Lidocaína	71-18	1
Fagron	Lidocaína	8J23-B02-3592391	1
Fagron	Lidocaína	B01-3635001	1
Fagron	Lidocaína	B01-3635002	1
Fagron	Lidocaína	B01-3635004	3
Fagron	Lidocaína	B01-3635006	2
Fagron	Lidocaína	B07-318310	1
Fagron	Lidocaína	F01-3763507	1
Fagron	Lidocaína	F03-3735001	1
Fagron	Lidocaína	F0-37349	1
Fagron	Lidocaína	F04-3698104	1
Fagron	Lidocaína	F04-3698105	2
Fagron	Lidocaína	F04-3698106	3
Fagron	Lidocaína	F04-3734907	1
Fagron	Lidocaína	F04-3734909	2
Fagron	Lidocaína	LDB/116049	2
Fagron	Lidocaína	LDB/117049	1
Fagron	Lidocaína	LDB/117093	4
Fagron	Lidocaína	LDB/118066	2
Fagron	Lidocaína	LDB/119043	5
Fagron	Lidocaína	LDB/119043x3	1
Fagron	Lidocaína	ldb/120006	1
Fagron	Lidocaína	LDB/120006	3
Fagron	Lidocaína	LDB/120018	2
Fagron	Lidocaína	LDB/722005	3
Fargon/ Sanacorp Lübeck	Lidocaína	18J23-B02-359237	1
Fargon/AHD	Lidocaína	17K23-B04-353428	1
Fargon/AHD	Lidocaína	18J23-B02-359238	1
Fargon/Fönix	Lidocaína	20C13-F04-369814	1
Fargon/Noweda	Lidocaína	17K23-B04-350543	1
Fargon/Noweda	Lidocaína	19F27-B01	1
Fargon/Phoenix	Lidocaína	13H05-N05	3
Fargon	Lidocaína	12E30-N10	1
Fargron	Lidocaína	14E13-B05-295552	1
Faron/Alliance	Lidocaína	16F21-B06-323670	2
Fragon/ Gehe	Lidocaína	19F27-B01-363502	1
Gatt-Koller	Lidocaína	1900471	1
GEHE 02.12.2014	Lidocaína	13J30-B02-292220	1
Gehe am 22.01.2014	Lidocaína	13H05-N05	2
Gehe Kassel	Lidocaína	14E13-B05-295550	1
Gehe	Lidocaína	12H16-N05	1
Gehe	Lidocaína	13B27-N04	1
Gehe	Lidocaína	14E13-B05-295552	1
GEHE	Lidocaína	16289503	1
Gehe	Lidocaína	16F21-B06-323670	1
GEHE	Lidocaína	16F21-B06-328421	1
Gehe	Lidocaína	17G03-B08-338286	2
Gehe	Lidocaína	17K23-B04-355709	1
GEHE	Lidocaína	18044405	1
Gehe	Lidocaína	18J23-B02-359239	1
Gehe	Lidocaína	19054505	2
Gehe	Lidocaína	192758005	2
Gehe	Lidocaína	20C13F04369816	1
Gehe	Lidocaína	22000398011	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Lidocaína	22000398016	1
Gehe	Lidocaína	22C15-B17-216739	1
Gehe	Lidocaína	23D25-B10-230220	1
Gehe	Lidocaína	23D25-B10-230226	1
GEHE	Lidocaína	23D25-B10-234510	1
Gehe	Lidocaína	23H23-B01-234506	1
Geilenkirchen	Lidocaína	17G03-B08-341306	1
Geilenkirchen	Lidocaína	LDB/117093	1
Geilenkirchen	Lidocaína	LDB/118066	1
GUMO	Lidocaína	19F27-B01-3635006	2
Gutenberg-Apotheke	Lidocaína	13J30-B02	1
Hedinger/Gehe	Lidocaína	17K23-B04-343250	1
Henry Lamotte Oils GmbH	Lidocaína		1
Jenne	Lidocaína	20003343015	1
Jenne	Lidocaína	2101035-02	1
Kehr	Lidocaína	16F21-B06-328421	1
Kehr	Lidocaína	16F21-B06-332251	1
Kehr	Lidocaína	17G03-B08-338284	1
Kehr	Lidocaína	22000398013	1
Kehr	Lidocaína	22C15-B17-216739	1
LaVita	Lidocaína	15H27-B07-318310	1
Moehs BCN S.L. / Noweda	Lidocaína	15332305	1
Nachprüfung von Juni 2018	Lidocaína	12C08-N11	1
Noweda	Lidocaína	10129901	1
Noweda	Lidocaína	12H16-N05	3
Noweda	Lidocaína	12H16-No5	1
Noweda	Lidocaína	16F21-B06	1
Noweda	Lidocaína	17K23-B04-347473	1
Noweda	Lidocaína	17K23-B04-350542	1
Noweda	Lidocaína	18044402	1
Noweda	Lidocaína	18J23-B02-355708	3
Noweda	Lidocaína	19054503	1
Noweda	Lidocaína	192758005	1
Noweda	Lidocaína	2003343016	1
Noweda	Lidocaína	220003908013	1
Noweda	Lidocaína	22000398013	1
Pharmachem	Lidocaína	17K23-B04-350541	1
PHOENIX 22.08.2014	Lidocaína		2
PHOENIX 22.08.2014	Lidocaína	13J30-B02-287640	1
Phoenix	Lidocaína	15332305	1
phoenix	Lidocaína	17348503	1
Phoenix	Lidocaína	17K23-B04-350543	1
Phoenix	Lidocaína	17K23-B05-345948	1
Phoenix	Lidocaína	18J23-B02-359238	1
Phoenix	Lidocaína	1905004-01	1
Phoenix	Lidocaína	19054504	1
Phoenix	Lidocaína	19f27-b01	1
Phoenix	Lidocaína	20003343004	1
Phoenix	Lidocaína	20004099001	1
Phoenix	Lidocaína	20c13-f04-369815	1
Phoenix	Lidocaína	20h13-f03-373501	1
Phoenix	Lidocaína	20H13-F04-373497	1
Phönix Gotha	Lidocaína	15A15-B01-304284	1
Phönix	Lidocaína	13352405	1
Phönix	Lidocaína	13B27-N04	1
Phönix	Lidocaína	17K23-B04-343250	1
Phönix	Lidocaína	17K23-B04-345215	1
Phönix	Lidocaína	17K23-B04-347475	1
Phönix	Lidocaína	19F27-B01-363505	1
Phönix	Lidocaína	2006013-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Lidocaína	200860209	1
PHönix	Lidocaína	20h13-f04-373499	1
Rondell Apotheke	Lidocaína	15332304	1
Sanacorp	Lidocaína	12H16-N05	1
Sanacorp	Lidocaína	12I21-N06	1
Sanacorp	Lidocaína	1603027-02	1
Sanacorp	Lidocaína	17183109	1
Sanacorp	Lidocaína	17K23-B04-350542	1
Sanacorp	Lidocaína	22000398011	2
Sanacorp	Lidocaína	22000398013	1
Sanacorp	Lidocaína	226002-01	1
Sanacorp	Lidocaína	22C15-B17-225236	1
Sanacorp	Lidocaína	22C15-B17-225237	3
Sanacorp	Lidocaína	23D25-B10-230221	1
Spangropharm	Lidocaína	18044410	1
Swati Pentose/ Link ...	Lidocaína	B2185	1
Swati Spentose / Gehe	Lidocaína	18J23-B02-359237	1
Swati Spentose / Gehe	Lidocaína	19F27-B01-363500	1
Swati Spentose / Gehe	Lidocaína	B01-3635001	1
SWATI SPENTOSE PRIVATE	Lidocaína	2101035-03	2
Swati Spentose Pvt L...	Lidocaína	B2185	1
Swati Spentose Pvt.L...	Lidocaína	21B10-B07213330	1
Swati Spentose Pvt.L...	Lidocaína	21B10-B07-213330	1
SWATI/Noweda	Lidocaína	LDB/119024	1
Swato Spentosen/Phoenix	Lidocaína	F04-3698105	1

- 234 339 spectra from 1515 *Apo-Ident* customers from a total of 48 845 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lidocaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lidocaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	600	0	201 484
Type C	0	1718	10	234 339

The substance/substance group *Lidocaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.4213 % (> 99.2477 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20942	20942	0,00	165,68
21640	24031	12,94	164,79
21673	24031	29,42	166,65
22984	22984	0,00	164,26
23019	22984	6,32	164,00
24031	24031	0,00	165,86
24928	24928	0,00	164,61
25533	25533	0,00	163,46
26654	26654	0,00	163,44

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**L-treonina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20734-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

L-treonina; Threoninum; Treonina levógira

Special notes

When selecting the *L-treonina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
L-treonina	7	8	4

Second-stage model

For differentiation of the substance/substance group *L-treonina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *L-treonina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato do ácido 5-aminolevulínico	78,62	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *L-treonina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *L-treonina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	L-treonina	1210027-01	21033	40	1403152
Euro OTC	L-treonina	1210027-01	22319	60	20121108
Euro OTC	L-treonina	1601031	22378	40	20160225*
Euro OTC	L-treonina	1909003	24850	40	20190913*
Euro OTC	L-treonina	2004005	25145	40	20200506*
Euro OTC	L-treonina	2011021	25468	40	20201210*
Euro OTC	L-treonina	2304006	26643	40	20230510*
Euro OTC	L-treonina	2304006	26643SI	20	20230510*
Fagron	L-treonina	12H02-N03	20734	40	1402580

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *L-treonina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 350 spectra of 10 reference samples from the substance/substance group *L-treonina*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-treonina	1606019	22679	40
Euro OTC	L-treonina	1609014	22792	40
Euro OTC	L-treonina	1703035	23158	40
Euro OTC	L-treonina	1711010	23738	40
Euro OTC	L-treonina	1811030	24417	40
Euro OTC	L-treonina	2201020	25946	40
Euro OTC	L-treonina	2208023	26522	40
Euro OTC	L-treonina	2404016	27279	40
Euro OTC	L-treonina	2201020	25946SI	10
Euro OTC	L-treonina	2208023	26522SI	20

- 201 734 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *L-treonina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	L-treonina	1606019-02	1
Euro OTC	L-treonina	1811030-01	1
Euro OTC	L-treonina	2011021-01	1
Fargon	L-treonina	2114720407	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *L-treonina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-treonina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	350	0	201 734
Type C	0	4	0	236 063

The substance/substance group *L-treonina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20734	20734	0,00	137,08
21033	21033	0,00	135,50
22319	25468	10,68	137,04

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22378	22378	0,00	138,01
24850	24850	0,00	136,10
25145	25145	0,00	141,57
25468	25468	0,00	134,86
26643	26643	0,00	138,08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Macrogol 1500**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20112-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Macrogol 1500; Macrogolum 1500; PEG 1500; Polietilenoglicol 1500

Special notes

When selecting the *Macrogol 1500* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Macrogol 1500	9	6	45

Second-stage model

For differentiation of the substance/substance group *Macrogol 1500* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Macrogol 1500* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Macrogol 4000	36,90	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Macrogol 1500* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Macrogol 1500*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol 1500	12324607	20977	40	1403323
Caelo	Macrogol 1500	17120001	23241	40	20170519
Caelo	Macrogol 1500	171200	23291	40	20170519*
Caelo	Macrogol 1500	21003420001	25988	40	20220103
Caelo	Macrogol 1500	21003420001	25988SI	30	20220103
Caelo	Macrogol 1500	24001044	27236	40	20240618*
Caelo	Macrogol 1500	24001044	27236SI	20	20240618*
Caelo	Macrogol 1500	24001643	27323	40	20240808*
Caelo	Macrogol 1500	24001643	27323SI	20	20240808*
Euro OTC	Macrogol 1500	1508002	21948	60	20150810*
Euro OTC	Macrogol 1500	1604005	22544	40	20160512*
Euro OTC	Macrogol 1500	2009003	25302	40	20200916*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 450 spectra of 12 reference samples from the substance/substance group *Macrogol 1500*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 512 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Macrogol 1500*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol 1500	172221	23625	40
Caelo	Macrogol 1500	182290	24350	40
Euro OTC	Macrogol 1500	1705004	23423	40
Euro OTC	Macrogol 1500	1705036	23440	40
Euro OTC	Macrogol 1500	1711032	23898	40
Euro OTC	Macrogol 1500	1806015	24147	40

- 201 844 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 85 spectra from 36 *Apo-Ident* customers from 47 batches from the substance/substance group *Macrogol 1500*.

- Among them are spectra of independent samples from 45 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
ACM / Herba	Macrogol 1500	KN-0826/10	1
Caelo	Macrogol 1500	10105901	1
Caelo	Macrogol 1500	11071309	1
Caelo	Macrogol 1500	12109409	1
Caelo	Macrogol 1500	13140901	1
Caelo	Macrogol 1500	13140902	2
Caelo	Macrogol 1500	13140906	1
Caelo	Macrogol 1500	14072409	1
Caelo	Macrogol 1500	14072412	1
Caelo	Macrogol 1500	15120007	1
Caelo	Macrogol 1500	1513101	1
Caelo	Macrogol 1500	15413101	2
Caelo	Macrogol 1500	15413104	1
Caelo	Macrogol 1500	15413105	5
Caelo	Macrogol 1500	15413111	2
Caelo	Macrogol 1500	16138407	1
Caelo	Macrogol 1500	17120001	3
Caelo	Macrogol 1500	17120002	2
Caelo	Macrogol 1500	17120009	1
Caelo	Macrogol 1500	17120011	2
Caelo	Macrogol 1500	17120012	3
Caelo	Macrogol 1500	18045703	1
Caelo	Macrogol 1500	1812905	1
Caelo	Macrogol 1500	18129503	1
Caelo	Macrogol 1500	18129505	1
Caelo	Macrogol 1500	18129506	1
Caelo	Macrogol 1500	18229002	2
Caelo	Macrogol 1500	18229004	2
Caelo	Macrogol 1500	192333501	1
Caelo	Macrogol 1500	19233501	3
Caelo	Macrogol 1500	20000729002	1
Caelo	Macrogol 1500	20000729005	1
Caesar & Loretz GmbH...	Macrogol 1500	21003420001	1
Caesar & Loretz GmbH	Macrogol 1500	19233501	1
Caesar & Loretz GmbH	Macrogol 1500	19233502	1
Caesar & Loretz GmbH	Macrogol 1500	20000729004	1
Caesar & Loretz GmbH	Macrogol 1500	21001042001	1
Caesar & Loretz GmbH	Macrogol 1500	21001042002	2
Caesar & Loretz GmbH	Macrogol 1500	21003420007	1
Euro OTC	Macrogol 1500	1103017-02	4
Euro OTC	Macrogol 1500	1206005-01	5
Euro OTC	Macrogol 1500	1304023-01	7
Euro OTC	Macrogol 1500	1406004-01	2
Euro OTC	Macrogol 1500	1503026-01	4
Euro OTC	Macrogol 1500	1806015-01	1
Euro OTC	Macrogol 1500	2009003-01	1
Gehe	Macrogol 1500	14072409	1
Krieger	Macrogol 1500	1712002	1
phoenix	Macrogol 1500	18229004	1
Phönix	Macrogol 1500	14072402	1

- 235 982 spectra from 1515 *Apo-Ident* customers from a total of 49 212 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Macrogol 1500* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Macrogol 1500* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	450	0	152 512
Type B	0	240	0	201 844
Type C	0	85	0	235 982

The substance/substance group *Macrogol 1500* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.9412 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20977	20977	0,00	65,25
21948	21948	0,00	88,41
22544	22544	0,00	117,62
23241	23291	10,88	56,72
23291	23291	0,00	57,01
25302	25302	0,00	68,17
25988	23291	6,41	54,98
27236	27236	0,00	91,78
27323	27323	0,00	68,89

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Macrogol 4000**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20690-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Macrogol 4000; PEG 4000; Polietilenoglicol 4000

Special notes

When selecting the *Macrogol 4000* substance/substance group, the following information is displayed to the user:

- Nota sobre como diferenciar do Macrogol 6000: O Macrogol 4000 não pode ser claramente diferenciado do Macrogol 6000, mas atualmente não está disponível comercialmente na Alemanha. Defina se é necessário fazer uma análise adicional.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Macrogol 4000	15	36	583

Second-stage model

For differentiation of the substance/substance group *Macrogol 4000* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Macrogol 4000* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Macrogol 1500	35,91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Macrogol 4000* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Macrogol 4000*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol 4000	12074116	20690	40	1401164
Caelo	Macrogol 4000	12318019	20975	40	1403322
Caelo	Macrogol 4000	12361502	21065	40	20130107
Caelo	Macrogol 4000	13356616	21357	40	20131107
Euro OTC	Macrogol 4000	1507004	21841	60	0000010550
Euro OTC	Macrogol 4000	1508031	21903	60	20150914*
Euro OTC	Macrogol 4000	1605012	22567	40	20160606*
Euro OTC	Macrogol 4000	1605025	22570	40	20160603*
Euro OTC	Macrogol 4000	1702003	23174	40	20170301*
Euro OTC	Macrogol 4000	1711016	23902	40	20171214*
Euro OTC	Macrogol 4000	2009016	25414	40	20200928*
Euro OTC	Macrogol 4000	2104009	25713	50	20210624*
Euro OTC	Macrogol 4000	2207019	26262	40	20220728*
Euro OTC	Macrogol 4000	2207019	26262SI	20	20220728*
Fagron	Macrogol 4000	15B13-B04-305461	21886	60	AR-16-FG-004020-01
Fagron	Macrogol 4000	16F10-B04-325645	23021	40	20160822

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 690 spectra of 16 reference samples from the substance/substance group *Macrogol 4000*. These samples are listed above in the *calibration samples* section. The reference samples come from 15 different batches.

- 152 272 spectra from a total of 2827 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1490 spectra of 39 reference samples from the substance/substance group *Macrogol 4000*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol 4000	11172433	20692	40
Caelo	Macrogol 4000	170686	23280	40
Caelo	Macrogol 4000	171190	23282	40
Caelo	Macrogol 4000	172081	23657	40
Caelo	Macrogol 4000	173039	23825	40
Caelo	Macrogol 4000	181974	24227	40
Caelo	Macrogol 4000	182154	24229	40
Caelo	Macrogol 4000	182448	24352	40
Caelo	Macrogol 4000	183153	24360	40
Caelo	Macrogol 4000	190093	24564	40
Caelo	Macrogol 4000	191756	24743	40
Caelo	Macrogol 4000	21001852005	26317	30
Caelo	Macrogol 4000	22003823	26477	40
Caelo	Macrogol 4000	22003814	26496	40
Caelo	Macrogol 4000	23000401	26691	40
Caelo	Macrogol 4000	24001280	27234	40
Caelo	Macrogol 4000	24002011	27445	40
Caelo	Macrogol 4000	24002115	27449	40
Euro OTC	Macrogol 4000	1609018	22791	40
Euro OTC	Macrogol 4000	1701007	22983	40
Euro OTC	Macrogol 4000	1705019	23433	40
Euro OTC	Macrogol 4000	1707026	23537	40
Euro OTC	Macrogol 4000	1804001	24089	40
Euro OTC	Macrogol 4000	1803029	24094	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Macrogol 4000	1810003	24339	40
Euro OTC	Macrogol 4000	1902009	24463	40
Euro OTC	Macrogol 4000	1907002	24798	40
Euro OTC	Macrogol 4000	1911027	25073	40
Euro OTC	Macrogol 4000	2007005	25326	40
Euro OTC	Macrogol 4000	2109002	25820	50
Euro OTC	Macrogol 4000	2207018	26276	40
Euro OTC	Macrogol 4000	2211018	26524	40
Euro OTC	Macrogol 4000	2401006	27153	40
Euro OTC	Macrogol 4000	2408012	27403	40
Fagron	Macrogol 4000	22A15-B06-216742	26071	40
Fagron	Macrogol 4000	24A19-B01-235824	27385	40
Caelo	Macrogol 4000	21001852005	26317SI	20
Euro OTC	Macrogol 4000	2207018	26276SI	20
Fagron	Macrogol 4000	22A15-B06-216742	26071SI	10

- 200 594 spectra from a total of 4009 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2313 spectra from 575 *Apo-Ident* customers from 591 batches from the substance/substance group *Macrogol 4000*.

- Among them are spectra of independent samples from 583 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Macrogol 4000	22001587006	1
	Macrogol 4000	22001929004	1
	Macrogol 4000	22003814008	1
	Macrogol 4000	22003814011	3
	Macrogol 4000	22003823005	6
	Macrogol 4000	22004211004	3
	Macrogol 4000	22004211006	2
	Macrogol 4000	22004211008	1
	Macrogol 4000	22004212003	4
	Macrogol 4000	22004213003	2
	Macrogol 4000	22004213004	3
	Macrogol 4000	22004213005	6
	Macrogol 4000	23001960006	1
	Macrogol 4000	23001960007	2
	Macrogol 4000	23001960008	7
	Macrogol 4000	23001960010	3
	Macrogol 4000	23002714002	2
	Macrogol 4000	23002714003	2
	Macrogol 4000	23002714004	2
	Macrogol 4000	23002741005	1
	Macrogol 4000	23C08-B02-228457	9
	Macrogol 4000	23C08-B02-229898	3
	Macrogol 4000	23C16-B18-229946	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Macrogol 4000	23C16-B18-229947	12
	Macrogol 4000	23C16-B18-2302203	1
	Macrogol 4000	23C16-B18-230223	1
	Macrogol 4000	24000623002	1
	Macrogol 4000	24000623006	1
	Macrogol 4000	24001280006	1
ACM	Macrogol 4000	KNC0366J15	2
AHC	Macrogol 4000	19000679007	1
AHC	Macrogol 4000	22004211001	1
AHD/Caesar & Loretz GmbH	Macrogol 4000	21001852005	1
AHD	Macrogol 4000	11H11-B05340782	1
AHD	Macrogol 4000	14L12-B06-301991	2
AHD	Macrogol 4000	15G15B07-313592	1
AHD	Macrogol 4000	16K25-B02-330527	3
AHD	Macrogol 4000	17208106	1
AHD	Macrogol 4000	17E02-B03	1
AHD	Macrogol 4000	17E02-B03-335507	3
AHD	Macrogol 4000	17K06-B05	2
AHD	Macrogol 4000	17K06-B05-345076	1
AHD	Macrogol 4000	18G30-B01	2
AHD	Macrogol 4000	18G30-B01-352394	2
AHD	Macrogol 4000	19000679005	1
AHD	Macrogol 4000	20001517005	1
AHD	Macrogol 4000	22004211006	1
AHD	Macrogol 4000	22004213005	1
AHD	Macrogol 4000	2211018-02	1
AHD	Macrogol 4000	23001960008	2
AHD	Macrogol 4000	23002714002	1
AHD	Macrogol 4000	23C16-B18-229946	1
AHD	Macrogol 4000	23C16-B18-229947	1
Alliance Healthcare	Macrogol 4000	12361512	2
Alliance	Macrogol 4000	18215403	1
Alliance	Macrogol 4000	20H21-F16-374090	1
Alliance	Macrogol 4000	21003792003	2
Alliance	Macrogol 4000	2109002-01	2
Alliance	Macrogol 4000	22001587010	3
Alliance	Macrogol 4000	22004211004	2
alliance	Macrogol 4000	23001960009	1
ANZAG 15.05.2014	Macrogol 4000	13356616	1
Anzag	Macrogol 4000	17068603	1
Audor Pharma	Macrogol 4000	2207018-01	2
Bombastus	Macrogol 4000	13136016	1
caedo	Macrogol 4000	17303902	2
Caelo	Macrogol 4000		1
Caelo	Macrogol 4000	1(20001517003)	1
Caelo	Macrogol 4000	1(20003397010)	1
Caelo	Macrogol 4000	1010023-02	1
Caelo	Macrogol 4000	1030517	1
Caelo	Macrogol 4000	11172303	1
Caelo	Macrogol 4000	1131117/16358107	1
Caelo	Macrogol 4000	1172404	1
Caelo	Macrogol 4000	1180513	1
Caelo	Macrogol 4000	1200617/16368105	1
Caelo	Macrogol 4000	12074102	1
Caelo	Macrogol 4000	12074109	3
Caelo	Macrogol 4000	12074114	1
Caelo	Macrogol 4000	12074116	3
Caelo	Macrogol 4000	12149108	1
Caelo	Macrogol 4000	12149113	2
Caelo	Macrogol 4000	12318011	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4000	12318019	1
Caelo	Macrogol 4000	12318027	1
Caelo	Macrogol 4000	1234	1
Caelo	Macrogol 4000	12345	1
Caelo	Macrogol 4000	1234Test	1
Caelo	Macrogol 4000	12361502	3
Caelo	Macrogol 4000	12361506	3
Caelo	Macrogol 4000	12361512	2
Caelo	Macrogol 4000	12361513	3
Caelo	Macrogol 4000	12361518	3
Caelo	Macrogol 4000	123test	1
Caelo	Macrogol 4000	123Test	1
Caelo	Macrogol 4000	1260917/16358105	1
Caelo	Macrogol 4000	13081501	1
Caelo	Macrogol 4000	13136001	3
Caelo	Macrogol 4000	13136003	3
Caelo	Macrogol 4000	13136009	3
Caelo	Macrogol 4000	13136010	1
Caelo	Macrogol 4000	13136011	4
Caelo	Macrogol 4000	1316003	1
Caelo	Macrogol 4000	13335102	1
Caelo	Macrogol 4000	13335106	1
Caelo	Macrogol 4000	13335107	1
Caelo	Macrogol 4000	13335120	1
Caelo	Macrogol 4000	13356601	4
Caelo	Macrogol 4000	13356602	3
Caelo	Macrogol 4000	13356609	1
Caelo	Macrogol 4000	13356611	4
Caelo	Macrogol 4000	13356616	1
Caelo	Macrogol 4000	13356617	6
Caelo	Macrogol 4000	13356621	1
Caelo	Macrogol 4000	1401708	1
Caelo	Macrogol 4000	14061705	5
Caelo	Macrogol 4000	14061707	4
Caelo	Macrogol 4000	14061708	9
Caelo	Macrogol 4000	14061713	1
Caelo	Macrogol 4000	14180503	1
Caelo	Macrogol 4000	14180504	1
Caelo	Macrogol 4000	14180508	2
Caelo	Macrogol 4000	14180511	2
Caelo	Macrogol 4000	14180520	4
Caelo	Macrogol 4000	14180522	1
Caelo	Macrogol 4000	14180524	1
Caelo	Macrogol 4000	14180525	3
Caelo	Macrogol 4000	14196007	1
Caelo	Macrogol 4000	14196013	1
Caelo	Macrogol 4000	14196017	1
Caelo	Macrogol 4000	143526	1
Caelo	Macrogol 4000	14352606	2
Caelo	Macrogol 4000	14352607	2
Caelo	Macrogol 4000	14352608	1
Caelo	Macrogol 4000	14352611	2
Caelo	Macrogol 4000	14352613	5
Caelo	Macrogol 4000	14352614	1
Caelo	Macrogol 4000	14352618	2
Caelo	Macrogol 4000	14J03-B07-304700	3
Caelo	Macrogol 4000	1508031-02	1
Caelo	Macrogol 4000	15159502	3
Caelo	Macrogol 4000	15159504	3
Caelo	Macrogol 4000	15159514	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4000	15159515	4
Caelo	Macrogol 4000	15159516	1
Caelo	Macrogol 4000	1517003	1
Caelo	Macrogol 4000	15225001	1
Caelo	Macrogol 4000	15225003	4
Caelo	Macrogol 4000	15225013	1
Caelo	Macrogol 4000	15335001	10
Caelo	Macrogol 4000	15335002	3
Caelo	Macrogol 4000	15335003	6
Caelo	Macrogol 4000	15335004	1
Caelo	Macrogol 4000	15335007	4
Caelo	Macrogol 4000	1535004	1
Caelo	Macrogol 4000	15376503	3
Caelo	Macrogol 4000	15376515	1
Caelo	Macrogol 4000	15376518	1
Caelo	Macrogol 4000	15376519	1
Caelo	Macrogol 4000	15406301	9
Caelo	Macrogol 4000	15406302	2
Caelo	Macrogol 4000	15406303	4
Caelo	Macrogol 4000	15406306	2
Caelo	Macrogol 4000	16023903	5
Caelo	Macrogol 4000	16023904	4
Caelo	Macrogol 4000	16023905	4
Caelo	Macrogol 4000	16023907	1
Caelo	Macrogol 4000	160912M	1
Caelo	Macrogol 4000	161017M/15406304	1
Caelo	Macrogol 4000	161202M/16152004	1
Caelo	Macrogol 4000	16152001	16
Caelo	Macrogol 4000	16152002	2
Caelo	Macrogol 4000	16152003	4
Caelo	Macrogol 4000	16267305	9
Caelo	Macrogol 4000	16267307	16
Caelo	Macrogol 4000	16267308	3
Caelo	Macrogol 4000	16267308/170227M	1
Caelo	Macrogol 4000	16267311	6
Caelo	Macrogol 4000	16308902	11
Caelo	Macrogol 4000	16308904	7
Caelo	Macrogol 4000	16308905	3
Caelo	Macrogol 4000	16308907	13
Caelo	Macrogol 4000	16308908	4
Caelo	Macrogol 4000	16358101	2
Caelo	Macrogol 4000	16358106	3
Caelo	Macrogol 4000	16358107	1
Caelo	Macrogol 4000	16358107/1111217	1
Caelo	Macrogol 4000	170105M16152004	1
Caelo	Macrogol 4000	170324M/16267308	1
Caelo	Macrogol 4000	17035603	2
Caelo	Macrogol 4000	17035604	4
Caelo	Macrogol 4000	17035606	13
Caelo	Macrogol 4000	17035607	5
Caelo	Macrogol 4000	17035608	1
Caelo	Macrogol 4000	170504M/16308906	1
Caelo	Macrogol 4000	170529M/16267308	1
Caelo	Macrogol 4000	170612M/17035603	1
Caelo	Macrogol 4000	17068603	4
Caelo	Macrogol 4000	170710M/17035603	1
Caelo	Macrogol 4000	170817M/17035603	1
Caelo	Macrogol 4000	170928M/17119002	1
Caelo	Macrogol 4000	171103M/17119002	1
Caelo	Macrogol 4000	17119001	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4000	17119005	2
Caelo	Macrogol 4000	171211M/17119003	1
Caelo	Macrogol 4000	17185601	2
Caelo	Macrogol 4000	1720103	1
Caelo	Macrogol 4000	17208103	13
Caelo	Macrogol 4000	17208104	24
Caelo	Macrogol 4000	17208105	2
Caelo	Macrogol 4000	17208106	2
Caelo	Macrogol 4000	1720813	1
Caelo	Macrogol 4000	17303901	18
Caelo	Macrogol 4000	17303902	9
Caelo	Macrogol 4000	17303903	1
Caelo	Macrogol 4000	17303905	1
Caelo	Macrogol 4000	17337901	6
Caelo	Macrogol 4000	17337902/1250418	1
Caelo	Macrogol 4000	17337902/1300518	1
Caelo	Macrogol 4000	17337902/2190218	1
Caelo	Macrogol 4000	17337906	1
Caelo	Macrogol 4000	177337906	1
Caelo	Macrogol 4000	18106101	2
Caelo	Macrogol 4000	18106103	5
Caelo	Macrogol 4000	18106104	6
Caelo	Macrogol 4000	18106105	34
Caelo	Macrogol 4000	18106106	9
Caelo	Macrogol 4000	18106109	5
Caelo	Macrogol 4000	18106110	4
Caelo	Macrogol 4000	18215403	4
Caelo	Macrogol 4000	18215404	5
Caelo	Macrogol 4000	18215405	2
Caelo	Macrogol 4000	18244802	18
Caelo	Macrogol 4000	18244803	11
Caelo	Macrogol 4000	18244805	14
Caelo	Macrogol 4000	18244806	4
Caelo	Macrogol 4000	18244809	2
Caelo	Macrogol 4000	18315301	17
Caelo	Macrogol 4000	18315302	11
Caelo	Macrogol 4000	18315303	13
Caelo	Macrogol 4000	18315304	6
Caelo	Macrogol 4000	18315305	8
Caelo	Macrogol 4000	18315307	20
Caelo	Macrogol 4000	18K01-B01-356808	1
Caelo	Macrogol 4000	190000679004	1
Caelo	Macrogol 4000	19000379004	1
Caelo	Macrogol 4000	1900067007	1
Caelo	Macrogol 4000	190006790006	1
Caelo	Macrogol 4000	19000679004	8
Caelo	Macrogol 4000	19000679005	10
Caelo	Macrogol 4000	19000679006	10
Caelo	Macrogol 4000	19000679007	24
Caelo	Macrogol 4000	19000679009	5
Caelo	Macrogol 4000	1900067909	1
Caelo	Macrogol 4000	1900679005	1
Caelo	Macrogol 4000	19009302	4
Caelo	Macrogol 4000	19009303	5
Caelo	Macrogol 4000	19009305	6
Caelo	Macrogol 4000	19009308	3
Caelo	Macrogol 4000	19009312	2
Caelo	Macrogol 4000	19009313	1
Caelo	Macrogol 4000	19009314	3
Caelo	Macrogol 4000	190908001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4000	19090801	1
Caelo	Macrogol 4000	19090804	1
Caelo	Macrogol 4000	190920	1
Caelo	Macrogol 4000	19142401	20
Caelo	Macrogol 4000	19142402	9
Caelo	Macrogol 4000	19142403	20
Caelo	Macrogol 4000	19142404	4
Caelo	Macrogol 4000	19142407	1
Caelo	Macrogol 4000	19175603	6
Caelo	Macrogol 4000	19175604	4
Caelo	Macrogol 4000	19175605	6
Caelo	Macrogol 4000	19175606	16
Caelo	Macrogol 4000	19175607	4
Caelo	Macrogol 4000	192227702	1
Caelo	Macrogol 4000	192277002	5
Caelo	Macrogol 4000	19227701	9
Caelo	Macrogol 4000	19227702	23
Caelo	Macrogol 4000	19227703	7
Caelo	Macrogol 4000	19227704	1
Caelo	Macrogol 4000	19227705	1
Caelo	Macrogol 4000	2(20003397010)	1
Caelo	Macrogol 4000	200002443005	1
Caelo	Macrogol 4000	200003397002	1
Caelo	Macrogol 4000	200003397005	1
Caelo	Macrogol 4000	200003397013	1
Caelo	Macrogol 4000	200003882003	1
Caelo	Macrogol 4000	20001303003	3
Caelo	Macrogol 4000	20001303007	1
Caelo	Macrogol 4000	2000151003	1
Caelo	Macrogol 4000	20001517001	1
Caelo	Macrogol 4000	20001517002	1
Caelo	Macrogol 4000	20001517003	24
Caelo	Macrogol 4000	20001517004	9
Caelo	Macrogol 4000	20001517005	8
Caelo	Macrogol 4000	20001517006	15
Caelo	Macrogol 4000	20001517008	1
Caelo	Macrogol 4000	20001517009	1
Caelo	Macrogol 4000	20002443003	2
Caelo	Macrogol 4000	20002443004	13
Caelo	Macrogol 4000	20002443005	7
Caelo	Macrogol 4000	20002443006	2
Caelo	Macrogol 4000	20002443007	11
Caelo	Macrogol 4000	20002443008	9
Caelo	Macrogol 4000	20002443009	7
Caelo	Macrogol 4000	20002443010	20
Caelo	Macrogol 4000	20002446004	1
Caelo	Macrogol 4000	20002494004	1
Caelo	Macrogol 4000	20003397002	26
Caelo	Macrogol 4000	20003397003	3
Caelo	Macrogol 4000	20003397004	14
Caelo	Macrogol 4000	20003397005	5
Caelo	Macrogol 4000	20003397007	15
Caelo	Macrogol 4000	20003397009	9
Caelo	Macrogol 4000	20003397010	13
Caelo	Macrogol 4000	20003397011	5
Caelo	Macrogol 4000	20003397012	7
Caelo	Macrogol 4000	20003397013	4
Caelo	Macrogol 4000	20003397014	7
Caelo	Macrogol 4000	20003397104	1
Caelo	Macrogol 4000	20003827001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4000	20003827006	4
Caelo	Macrogol 4000	20003827011	3
Caelo	Macrogol 4000	20003882001	6
Caelo	Macrogol 4000	20003882002	16
Caelo	Macrogol 4000	20003882003	5
Caelo	Macrogol 4000	20003882005	2
Caelo	Macrogol 4000	2000397004	1
Caelo	Macrogol 4000	2000397014	1
Caelo	Macrogol 4000	2001517003	1
Caelo	Macrogol 4000	2003397013	1
Caelo	Macrogol 4000	200691307	1
Caelo	Macrogol 4000	210003792002	1
Caelo	Macrogol 4000	21001520001	1
Caelo	Macrogol 4000	2100152006	1
Caelo	Macrogol 4000	21001845001	7
Caelo	Macrogol 4000	21001845002	5
Caelo	Macrogol 4000	21001846001	7
Caelo	Macrogol 4000	21001850001	1
Caelo	Macrogol 4000	21001850003	14
Caelo	Macrogol 4000	21001850005	6
Caelo	Macrogol 4000	21001850007	7
Caelo	Macrogol 4000	21001852005	13
Caelo	Macrogol 4000	21001852006	5
Caelo	Macrogol 4000	21001852007	6
Caelo	Macrogol 4000	21001852008	1
Caelo	Macrogol 4000	21003792002	11
Caelo	Macrogol 4000	21003792003	4
Caelo	Macrogol 4000	21003792004	6
Caelo	Macrogol 4000	21003792005	6
Caelo	Macrogol 4000	21003792006	1
Caelo	Macrogol 4000	21003795003	1
Caelo	Macrogol 4000	210037992003	1
Caelo	Macrogol 4000	210906(2101845001)	1
Caelo	Macrogol 4000	210923(20003397010)	1
Caelo	Macrogol 4000	211019(21001846001)	1
Caelo	Macrogol 4000	211124(21001850005)	1
Caelo	Macrogol 4000	211215(21001850005)	1
Caelo	Macrogol 4000	22001201001	1
Caelo	Macrogol 4000	22001587004	1
Caelo	Macrogol 4000	22001587005	9
Caelo	Macrogol 4000	22001587006	4
Caelo	Macrogol 4000	22001587007	17
Caelo	Macrogol 4000	22001587010	3
Caelo	Macrogol 4000	22001587013	1
Caelo	Macrogol 4000	22001587014	2
Caelo	Macrogol 4000	22001587015	1
Caelo	Macrogol 4000	22003814005	1
Caelo	Macrogol 4000	22003814006	4
Caelo	Macrogol 4000	22003814007	1
Caelo	Macrogol 4000	22003814008	1
Caelo	Macrogol 4000	22003814009	5
Caelo	Macrogol 4000	22003814011	1
Caelo	Macrogol 4000	22003814012	5
Caelo	Macrogol 4000	22003814013	1
Caelo	Macrogol 4000	22003814014	3
Caelo	Macrogol 4000	22003823005	1
Caelo	Macrogol 4000	2200421003	1
Caelo	Macrogol 4000	22004211001	2
Caelo	Macrogol 4000	22004211002	1
Caelo	Macrogol 4000	22004211006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4000	22004213004	1
Caelo	Macrogol 4000	22004213005	1
Caelo	Macrogol 4000	220042163003	1
Caelo	Macrogol 4000	220117	1
Caelo	Macrogol 4000	220210(21001845001)	1
Caelo	Macrogol 4000	220210(21001852006)	1
Caelo	Macrogol 4000	220315(21003792002)	2
Caelo	Macrogol 4000	220412(21003792002)	1
Caelo	Macrogol 4000	220428(21003792002)	1
Caelo	Macrogol 4000	220516(21003792005)	1
Caelo	Macrogol 4000	220519(21003792005)	1
Caelo	Macrogol 4000	220804(22001587007)	1
Caelo	Macrogol 4000	220905(22001587014)	1
Caelo	Macrogol 4000	22A15-B06	1
Caelo	Macrogol 4000	23001960008	1
Caelo	Macrogol 4000	23001960009	1
Caelo	Macrogol 4000	23061505	1
Caelo	Macrogol 4000	24000623005	1
Caelo	Macrogol 4000	28111706	1
Caelo	Macrogol 4000	3(20003397010)	1
Caelo	Macrogol 4000	30041803	1
Caelo	Macrogol 4000	39393137	1
Caelo	Macrogol 4000	3940608	1
Caelo	Macrogol 4000	4123585	1
Caelo	Macrogol 4000	5041701	1
Caelo	Macrogol 4000	5406301	1
Caelo	Macrogol 4000	9061805	1
Caelo	Macrogol 4000	90908	1
Caelo	Macrogol 4000	IntCh217002	1
Caesar & Loretz GmbH...	Macrogol 4000	21003792003	3
Caesar & Loretz GmbH...	Macrogol 4000	22003814007	3
Caesar & Loretz GmbH...	Macrogol 4000	20001517003	1
Caesar & Loretz GmbH...	Macrogol 4000	18315307	1
Caesar & Loretz GmbH...	Macrogol 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogol 4000	19175606	1
Caesar & Loretz GmbH...	Macrogol 4000	22003823005	1
Caesar & Loretz GmbH...	Macrogol 4000	18315307	1
Caesar & Loretz GmbH...	Macrogol 4000	19142401	1
Caesar & Loretz GmbH/ AHD	Macrogol 4000	19009302	1
Caesar & Loretz GmbH...	Macrogol 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogol 4000	20003882002	1
Caesar & Loretz GmbH...	Macrogol 4000	21001845001	1
Caesar & Loretz GmbH...	Macrogol 4000	21001852005	1
Caesar & Loretz GmbH/AHD	Macrogol 4000	19009302	1
Caesar & Loretz GmbH/AHD	Macrogol 4000	20003397002	1
Caesar & Loretz GmbH/AHD	Macrogol 4000	20003397007	2
Caesar & Loretz GmbH/AHD	Macrogol 4000	20003397009	1
Caesar & Loretz GmbH/AHD	Macrogol 4000	22001587010	2
Caesar & Loretz GmbH/AHD	Macrogol 4000	22004211006	1
Caesar & Loretz GmbH...	Macrogol 4000	19000679005	3
Caesar & Loretz GmbH...	Macrogol 4000	19227703	2
Caesar & Loretz GmbH...	Macrogol 4000	20003397010	2
Caesar & Loretz GmbH...	Macrogol 4000	22001587014	1
Caesar & Loretz GmbH/E	Macrogol 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogol 4000	20001517003	1
Caesar & Loretz GmbH...	Macrogol 4000	20003397002	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	18244802	1
Caesar & Loretz GmbH/GEHE	Macrogol 4000	19000679004	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	19142401	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	20001303003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Macrogol 4000	20001517003	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	20003397003	1
Caesar & Loretz GmbH/gehe	Macrogol 4000	20003882001	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	20003882005	2
Caesar & Loretz GmbH/Gehe	Macrogol 4000	21001845001	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	21003792005	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	21003795003	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	22001587004	1
Caesar & Loretz GmbH/Gehe	Macrogol 4000	22003814014	2
Caesar & Loretz GmbH…	Macrogol 4000	20003882005	1
Caesar & Loretz GmbH…	Macrogol 4000	19000679004	1
Caesar & Loretz GmbH…	Macrogol 4000	20002443008	1
Caesar & Loretz GmbH…	Macrogol 4000	21001845001	2
Caesar & Loretz GmbH…	Macrogol 4000	21001852005	2
Caesar & Loretz GmbH…	Macrogol 4000	21003792002	1
Caesar & Loretz GmbH…	Macrogol 4000	22001587007	3
Caesar & Loretz GmbH…	Macrogol 4000	22004211006	1
Caesar & Loretz GmbH…	Macrogol 4000	22004213004	1
Caesar & Loretz GmbH…	Macrogol 4000	18315307	1
Caesar & Loretz GmbH…	Macrogol 4000	20003397012	1
Caesar & Loretz GmbH…	Macrogol 4000	21001846001	1
Caesar & Loretz GmbH…	Macrogol 4000	21001850005	2
Caesar & Loretz GmbH…	Macrogol 4000	21001852005	1
Caesar & Loretz GmbH/PH	Macrogol 4000	19000679007	1
Caesar & Loretz GmbH…	Macrogol 4000	20002443008	2
Caesar & Loretz GmbH/Phoe	Macrogol 4000	20003397011	1
Caesar & Loretz GmbH…	Macrogol 4000	19090804	2
Caesar & Loretz GmbH…	Macrogol 4000	20003397011	4
Caesar & Loretz GmbH…	Macrogol 4000	20003882005	1
Caesar & Loretz GmbH…	Macrogol 4000	22001587007	2
Caesar & Loretz GmbH…	Macrogol 4000	21001852006	2
Caesar & Loretz GmbH…	Macrogol 4000	21003792005	2
Caesar & Loretz GmbH…	Macrogol 4000	23001960008	3
Caesar & Loretz GmbH/Sana	Macrogol 4000	20002443010	1
Caesar & Loretz GmbH…	Macrogol 4000	18106105	1
Caesar & Loretz GmbH…	Macrogol 4000	20003397002	1
Caesar & Loretz GmbH…	Macrogol 4000	20003397012	2
Caesar & Loretz GmbH…	Macrogol 4000	22003814011	1
Caesar & Loretz GmbH	Macrogol 4000	14180520	1
Caesar & Loretz GmbH	Macrogol 4000	17337911	1
Caesar & Loretz GmbH	Macrogol 4000	18106105	2
Caesar & Loretz GmbH	Macrogol 4000	18244802	2
Caesar & Loretz GmbH	Macrogol 4000	18244803	1
Caesar & Loretz GmbH	Macrogol 4000	18244806	1
Caesar & Loretz GmbH	Macrogol 4000	18315301	2
Caesar & Loretz GmbH	Macrogol 4000	18315302	5
Caesar & Loretz GmbH	Macrogol 4000	18315303	3
Caesar & Loretz GmbH	Macrogol 4000	18315307	6
Caesar & Loretz GmbH	Macrogol 4000	19000679004	3
Caesar & Loretz GmbH	Macrogol 4000	19000679006	3
Caesar & Loretz GmbH	Macrogol 4000	19000679007	11
Caesar & Loretz GmbH	Macrogol 4000	19009302	3
Caesar & Loretz GmbH	Macrogol 4000	19009303	1
Caesar & Loretz GmbH	Macrogol 4000	19009305	2
Caesar & Loretz GmbH	Macrogol 4000	19009308	9
Caesar & Loretz GmbH	Macrogol 4000	19009313	2
Caesar & Loretz GmbH	Macrogol 4000	19142401	8
Caesar & Loretz GmbH	Macrogol 4000	19142402	3
Caesar & Loretz GmbH	Macrogol 4000	19142407	4
Caesar & Loretz GmbH	Macrogol 4000	19175605	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Macrogol 4000	19175606	9
Caesar & Loretz GmbH	Macrogol 4000	19175607	2
Caesar & Loretz GmbH	Macrogol 4000	192277002	1
Caesar & Loretz GmbH	Macrogol 4000	19227702	7
Caesar & Loretz GmbH	Macrogol 4000	19227703	1
Caesar & Loretz GmbH	Macrogol 4000	20001517003	7
Caesar & Loretz GmbH	Macrogol 4000	20001517006	1
Caesar & Loretz GmbH	Macrogol 4000	20001517009	1
Caesar & Loretz GmbH	Macrogol 4000	20002443004	2
Caesar & Loretz GmbH	Macrogol 4000	20002443005	2
Caesar & Loretz GmbH	Macrogol 4000	20002443007	1
Caesar & Loretz GmbH	Macrogol 4000	20002443008	2
Caesar & Loretz GmbH	Macrogol 4000	20002443010	6
Caesar & Loretz GmbH	Macrogol 4000	20002494004	1
Caesar & Loretz GmbH	Macrogol 4000	20003397002	9
Caesar & Loretz GmbH	Macrogol 4000	20003397003	2
Caesar & Loretz GmbH	Macrogol 4000	20003397004	1
Caesar & Loretz GmbH	Macrogol 4000	20003397007	6
Caesar & Loretz GmbH	Macrogol 4000	20003397010	1
Caesar & Loretz GmbH	Macrogol 4000	20003397012	4
Caesar & Loretz GmbH	Macrogol 4000	20003397013	6
Caesar & Loretz GmbH	Macrogol 4000	20003397014	8
Caesar & Loretz GmbH	Macrogol 4000	20003882001	1
Caesar & Loretz GmbH	Macrogol 4000	20003882002	1
Caesar & Loretz GmbH	Macrogol 4000	21001845002	1
Caesar & Loretz GmbH	Macrogol 4000	21001846001	5
Caesar & Loretz GmbH	Macrogol 4000	21001850005	1
Caesar & Loretz GmbH	Macrogol 4000	21001850007	2
Caesar & Loretz GmbH	Macrogol 4000	21001852005	1
Caesar & Loretz GmbH	Macrogol 4000	21001852006	4
Caesar & Loretz GmbH	Macrogol 4000	21001852007	3
Caesar & Loretz GmbH	Macrogol 4000	21001852008	1
Caesar & Loretz GmbH	Macrogol 4000	21003792002	7
Caesar & Loretz GmbH	Macrogol 4000	21003792004	5
Caesar & Loretz GmbH	Macrogol 4000	21003792005	9
Caesar & Loretz GmbH	Macrogol 4000	22001587004	2
Caesar & Loretz GmbH	Macrogol 4000	22001587005	4
Caesar & Loretz GmbH	Macrogol 4000	22001587006	4
Caesar & Loretz GmbH	Macrogol 4000	22001587007	3
Caesar & Loretz GmbH	Macrogol 4000	22003814007	1
Caesar & Loretz GmbH	Macrogol 4000	22003814008	2
Caesar & Loretz GmbH	Macrogol 4000	22003814009	2
Caesar & Loretz GmbH	Macrogol 4000	22003814011	2
Caesar & Loretz GmbH	Macrogol 4000	22003814013	2
Caesar & Loretz GmbH	Macrogol 4000	22003823005	1
Caesar & Loretz GmbH	Macrogol 4000	F16-3740901	1
Caesar & Loretz Hild…	Macrogol 4000	19000679007	1
Caesar&Loretz GmbH/ …	Macrogol 4000	17068603	1
Caesar&Loretz GmbH/Anzag	Macrogol 4000	14196017	1
Calo, Hilden/ Phönix	Macrogol 4000	19142401	1
calo	Macrogol 4000	17303902	1
Cealo / Anzag	Macrogol 4000	211020(21001846001)	1
Cealo / Anzag	Macrogol 4000	211115(21001846001)	1
Cealo / Anzag	Macrogol 4000	211217(21001850005)	1
Cealo/Anzag	Macrogol 4000	21001850005	1
Cealo/Gehe	Macrogol 4000	16023907	1
Cealo/Jenne	Macrogol 4000	220125(21001852006)	1
DIV GH	Macrogol 4000	13/12	1
EuRho	Macrogol 4000	1206009-01	1
Euro OTC	Macrogol 4000	1005011-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Macrogol 4000	1202040-02	2
Euro OTC	Macrogol 4000	130502002	1
Euro OTC	Macrogol 4000	1305020-02	4
Euro OTC	Macrogol 4000	140701001	1
Euro OTC	Macrogol 4000	1507004-01	1
Euro OTC	Macrogol 4000	1508031-01	1
Euro OTC	Macrogol 4000	1508031-02	1
Euro OTC	Macrogol 4000	15159515	1
Euro OTC	Macrogol 4000	1705019-01	1
Euro OTC	Macrogol 4000	1707026-01	1
Euro OTC	Macrogol 4000	1711016-01	1
Euro OTC	Macrogol 4000	17303905	1
Euro OTC	Macrogol 4000	1808003-01	4
Euro OTC	Macrogol 4000	1808003-02	5
Euro OTC	Macrogol 4000	180803-02	1
Euro OTC	Macrogol 4000	1810003-01	2
Euro OTC	Macrogol 4000	18315307	1
Euro OTC	Macrogol 4000	1902009-01	4
Euro OTC	Macrogol 4000	1911027-01	12
Euro OTC	Macrogol 4000	2007005-01	5
Euro OTC	Macrogol 4000	2009016-01	4
Euro OTC	Macrogol 4000	210400901	1
Euro OTC	Macrogol 4000	2104009-01	2
Euro OTC	Macrogol 4000	2109002-03	1
Euro OTC	Macrogol 4000	22/28	1
Euro OTC	Macrogol 4000	2207018-01	4
Euro OTC	Macrogol 4000	2211018-01	4
Facron	Macrogol 4000	7022014C	1
Fagron	Macrogol 4000	10022015A	1
Fagron	Macrogol 4000	10022015B	1
Fagron	Macrogol 4000	1112M-02103	1
Fagron	Macrogol 4000	123Test	1
Fagron	Macrogol 4000	12F13-N01	1
Fagron	Macrogol 4000	12F29-N01	2
Fagron	Macrogol 4000	12F29-NO1	1
Fagron	Macrogol 4000	12I20-n03	1
Fagron	Macrogol 4000	12L10-N06	2
Fagron	Macrogol 4000	13356608	1
Fagron	Macrogol 4000	13A10-N01	1
Fagron	Macrogol 4000	13B20N01	1
Fagron	Macrogol 4000	13B20-N01	2
Fagron	Macrogol 4000	13E22-N03	6
Fagron	Macrogol 4000	13F12N09	1
Fagron	Macrogol 4000	13F12-N09	1
Fagron	Macrogol 4000	13G19-N08	2
Fagron	Macrogol 4000	13G19-N14	1
Fagron	Macrogol 4000	13I17-N03	1
Fagron	Macrogol 4000	13I30-N03	1
Fagron	Macrogol 4000	13L30-B31	1
Fagron	Macrogol 4000	13l30-N03	1
Fagron	Macrogol 4000	14A03B01	1
Fagron	Macrogol 4000	14A03-B01-289602	3
Fagron	Macrogol 4000	14A03-B01-289605	1
Fagron	Macrogol 4000	14D14-B06	1
Fagron	Macrogol 4000	14D14-B06-293453	2
Fagron	Macrogol 4000	14G15-B07-295632	1
Fagron	Macrogol 4000	14G21-B04-296899	1
Fagron	Macrogol 4000	14J03-B07300840	1
Fagron	Macrogol 4000	14J03-B07-300840	1
Fagron	Macrogol 4000	14K03-_b07-300522	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Macrogol 4000	14K03-B07-300522	2
Fagron	Macrogol 4000	14L12-B06	1
Fagron	Macrogol 4000	15/29-B01-318038	2
Fagron	Macrogol 4000	15092014A	1
Fagron	Macrogol 4000	15376510	1
Fagron	Macrogol 4000	15A08-B03-302761	1
Fagron	Macrogol 4000	15A08B03302762	1
Fagron	Macrogol 4000	15A08-B03-302762	3
Fagron	Macrogol 4000	15b03-b08-304701	1
Fagron	Macrogol 4000	15B13-B04-305461	3
Fagron	Macrogol 4000	15G15-B07	1
Fagron	Macrogol 4000	15G15-B07-313592	2
Fagron	Macrogol 4000	15H10-B04-314037	2
Fagron	Macrogol 4000	15H10-B04-31407	1
Fagron	Macrogol 4000	15I29-B01-318038	1
Fagron	Macrogol 4000	160514a	1
Fagron	Macrogol 4000	16102013A	1
Fagron	Macrogol 4000	16152002	1
Fagron	Macrogol 4000	16A20-B15-320060	1
Fagron	Macrogol 4000	16a20-b15-320652	8
Fagron	Macrogol 4000	16A20-B15-320652	6
Fagron	Macrogol 4000	16F10-B04-324270	1
Fagron	Macrogol 4000	16K25-B02-330527	2
Fagron	Macrogol 4000	17012014A	1
Fagron	Macrogol 4000	17E02-B03-335507	1
Fagron	Macrogol 4000	17E02-BO3-335526	3
Fagron	Macrogol 4000	17H11-BO5-39499	1
Fagron	Macrogol 4000	17I11-BO1-341774	2
Fagron	Macrogol 4000	17K06-B05-345076	3
Fagron	Macrogol 4000	17K06-B05345096	1
Fagron	Macrogol 4000	17K06-B05-345096	2
Fagron	Macrogol 4000	1803029-01	2
Fagron	Macrogol 4000	18082014C	1
Fagron	Macrogol 4000	18D10-BO4-349676	1
Fagron	Macrogol 4000	18G30-B01	2
Fagron	Macrogol 4000	18G30-B01-345096	1
Fagron	Macrogol 4000	18K01-B01	1
Fagron	Macrogol 4000	18K01-B01-355299	1
Fagron	Macrogol 4000	19142403	1
Fagron	Macrogol 4000	19B06-B04	1
Fagron	Macrogol 4000	19B06-B04-359646	2
Fagron	Macrogol 4000	19B06-B04-359656	1
Fagron	Macrogol 4000	19G17-B03-363522	1
Fagron	Macrogol 4000	19H08-B03-364385	2
Fagron	Macrogol 4000	19H28-F07	1
Fagron	Macrogol 4000	19H28-F07-3643908	1
Fagron	Macrogol 4000	19H28-F07-364398	2
Fagron	Macrogol 4000	19H28-fo7-364388	1
Fagron	Macrogol 4000	19J28-F03	3
Fagron	Macrogol 4000	19J28-F03-366720	2
Fagron	Macrogol 4000	20/46	1
Fagron	Macrogol 4000	20002443007	1
Fagron	Macrogol 4000	20092014A	1
Fagron	Macrogol 4000	20122013C	1
Fagron	Macrogol 4000	2022015A	1
Fagron	Macrogol 4000	20803-F03-369765	1
Fagron	Macrogol 4000	20B03-F03	4
Fagron	Macrogol 4000	20B03-F03-369410	7
Fagron	Macrogol 4000	20B03-F03-369411	3
Fagron	Macrogol 4000	20B03-F03-369424	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Macrogol 4000	20B03-F03-369426	4
Fagron	Macrogol 4000	20B03-F03-369765	2
Fagron	Macrogol 4000	20E19-F01	1
Fagron	Macrogol 4000	20E19-F01-3718706	1
Fagron	Macrogol 4000	20E19-F01-371876	1
Fagron	Macrogol 4000	20E19-F01-371877	1
Fagron	Macrogol 4000	20-E19-F01-371877	1
Fagron	Macrogol 4000	20E19-F01-371878	1
Fagron	Macrogol 4000	20H21-F16	3
Fagron	Macrogol 4000	20H21-F16-374092	2
Fagron	Macrogol 4000	20H21-F16-374094	2
Fagron	Macrogol 4000	20K16-F05	2
Fagron	Macrogol 4000	20K16-F05-376031	3
Fagron	Macrogol 4000	20K16-F05-376034	1
Fagron	Macrogol 4000	21/37	2
Fagron	Macrogol 4000	21052015A	1
Fagron	Macrogol 4000	2122013a	1
Fagron	Macrogol 4000	2122013b	1
Fagron	Macrogol 4000	21B12-F03-377352	1
Fagron	Macrogol 4000	21B23-F01	2
Fagron	Macrogol 4000	21B23-F01-377361	2
Fagron	Macrogol 4000	21E8-B05-216626	1
Fagron	Macrogol 4000	21K08-B09-213154	1
Fagron	Macrogol 4000	22062015A	1
Fagron	Macrogol 4000	22122014A	1
Fagron	Macrogol 4000	2215I-02103	1
Fagron	Macrogol 4000	22A15_B06_216742	1
Fagron	Macrogol 4000	22A15-B06	1
Fagron	Macrogol 4000	22A15-B06-216677	2
Fagron	Macrogol 4000	22A15-B06-216742	2
Fagron	Macrogol 4000	22A15-B06-220791	5
Fagron	Macrogol 4000	22A25-B03-221082	3
Fagron	Macrogol 4000	22A25B03-221660	1
Fagron	Macrogol 4000	22A25-B03-221660	2
Fagron	Macrogol 4000	22A25-B03-224251	4
Fagron	Macrogol 4000	22G05-B01-221487	2
Fagron	Macrogol 4000	22G05-B01-223076	2
Fagron	Macrogol 4000	22G05-B01-224252	6
Fagron	Macrogol 4000	22L07-B02-225861	2
Fagron	Macrogol 4000	23C16-B18-229947	1
Fagron	Macrogol 4000	25082014A	1
Fagron	Macrogol 4000	25322-68-3	1
Fagron	Macrogol 4000	26052014A	1
Fagron	Macrogol 4000	26082013A	1
Fagron	Macrogol 4000	28052014B	1
Fagron	Macrogol 4000	280913C	2
Fagron	Macrogol 4000	2818A-02103	1
Fagron	Macrogol 4000	290714c	1
Fagron	Macrogol 4000	20B03-F03	2
Fagron	Macrogol 4000	30092014B	1
Fagron	Macrogol 4000	3032014B	1
Fagron	Macrogol 4000	30B03	1
Fagron	Macrogol 4000	3114I-02103	1
Fagron	Macrogol 4000	3217M-02103	1
Fagron	Macrogol 4000	505201C	1
Fagron	Macrogol 4000	701014	1
Fagron	Macrogol 4000	701014-0006	3
Fagron	Macrogol 4000	701014-0014	1
Fagron	Macrogol 4000	8012015A	1
Fagron	Macrogol 4000	8062015B	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Macrogol 4000	8062015C	1
Fagron	Macrogol 4000	914I-02103	1
Fagron	Macrogol 4000	F03-3667200	1
Fagron	Macrogol 4000	F07-3643808	1
Fagron	Macrogol 4000	F16-3740901	1
Fiebig	Macrogol 4000	13356601	1
Fiebig	Macrogol 4000	14180506	1
Fiebig	Macrogol 4000	15159514	1
Fiebig	Macrogol 4000	16152001	1
Fiebig	Macrogol 4000	16308907	1
Fiebig	Macrogol 4000	17035607	1
Finteler Apotheke	Macrogol 4000	16308907	2
Finteler Apotheke	Macrogol 4000	17035607	1
Gatt-Koller	Macrogol 4000	1420/04152915	1
Gatt-Koller	Macrogol 4000	1420/04153415	1
Gatt-Koller	Macrogol 4000	1802391	1
Gatt-Koller	Macrogol 4000	1804126	1
Gatt-Koller	Macrogol 4000	2792/07153315	1
Gatt-Koller	Macrogol 4000	4643/01170417	2
Gehe / EuRho	Macrogol 4000	1803029-01	1
GEHE 06.05.2014	Macrogol 4000	13356608	2
Gehe	Macrogol 4000	14K03-B07-300522	1
Gehe	Macrogol 4000	15159514	3
Gehe	Macrogol 4000	16267307	1
Gehe	Macrogol 4000	16308907	1
Gehe	Macrogol 4000	17208104	1
GEHE	Macrogol 4000	18106109	1
Gehe	Macrogol 4000	19009303	1
Gehe	Macrogol 4000	19142401	1
Gehe	Macrogol 4000	19175607	1
Gehe	Macrogol 4000	20001517003	2
Gehe	Macrogol 4000	21003795003	1
gehe	Macrogol 4000	22004213005	1
Gepepharm/ Gehe	Macrogol 4000	1508031-02	1
Gutenberg-Apotheke	Macrogol 4000	13356609	1
Hedinger	Macrogol 4000	13G19-N08	1
Henry Lamotte Oils GMBH	Macrogol 4000	16267308/170127M	1
Henry Lamotte/AHD	Macrogol 4000	17303901	1
Henry Lamotte	Macrogol 4000	1213test	1
Kehr	Macrogol 4000	16308907	1
Kehr	Macrogol 4000	18106105	1
Kehr	Macrogol 4000	22003823005	1
KÖGL	Macrogol 4000	1900232	1
Macgol 4000	Macrogol 4000	16267308	2
Macgol 4000	Macrogol 4000	16F10-B04	1
Nachprüfung	Macrogol 4000	14A03-B01-289605	1
Nachtestung-Verlängerung	Macrogol 4000	17/17	1
Noveda	Macrogol 4000	18315307	1
Noweda	Macrogol 4000	12361502	2
Noweda	Macrogol 4000	12361512	1
Noweda	Macrogol 4000	13136003	1
Noweda	Macrogol 4000	17303902	1
Noweda	Macrogol 4000	17E02-B03-335526	1
Noweda	Macrogol 4000	18106109	2
Noweda	Macrogol 4000	18315303	1
Noweda	Macrogol 4000	19H08-B03-364385	1
Noweda	Macrogol 4000	20001517003	1
Noweda	Macrogol 4000	20003397004	3
Noweda	Macrogol 4000	20003397010	1
Noweda	Macrogol 4000	20003397013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Macrogol 4000	21001850003	1
Noweda	Macrogol 4000	22001587007	3
Noweda	Macrogol 4000	22003814013	2
Noweda	Macrogol 4000	2200421001	1
Noweda	Macrogol 4000	22004211002	2
Noweda	Macrogol 4000	22004212003	3
Noweda	Macrogol 4000	22004213004	2
Noweda	Macrogol 4000	22A15B06216742	1
Noweda	Macrogol 4000	23001960009	1
Noweda	Macrogol 4000	2300196007	1
Noweda	Macrogol 4000	23C08-B02-227792	1
Phoenix	Macrogol 4000	12258901	1
Phoenix	Macrogol 4000	16023905	1
Phoenix	Macrogol 4000	18315307	2
Phoenix	Macrogol 4000	19175606	1
Phoenix	Macrogol 4000	20003397002	1
Phönix	Macrogol 4000	1202040-02	1
phönix	Macrogol 4000	1502031-02	1
phönix	Macrogol 4000	1535007	1
phönix	Macrogol 4000	15406302	1
phönix	Macrogol 4000	16023904	1
phönix	Macrogol 4000	1605012-01	1
phönix	Macrogol 4000	1701007-01	3
Phönix	Macrogol 4000	1707026-01	1
PHÖNIX	Macrogol 4000	19000679007	1
Phönix	Macrogol 4000	19142401	1
Phönix	Macrogol 4000	19142403	4
Phönix	Macrogol 4000	20002443004	1
Phönix	Macrogol 4000	20002443009	1
PHÖNIX	Macrogol 4000	20003397002	1
Phönix	Macrogol 4000	20003827011	1
Phönix	Macrogol 4000	23002714005	1
Rondell Apotheke	Macrogol 4000	16023905	1
Sanacorp	Macrogol 4000	14061707	1
Sanacorp	Macrogol 4000	15376520	1
Sanacorp	Macrogol 4000	17208104	1
Sanacorp	Macrogol 4000	17303901	1
Sanacorp	Macrogol 4000	18244802	1
Sanacorp	Macrogol 4000	19000679007	1
Sanacorp	Macrogol 4000	19142401	1
Sanacorp	Macrogol 4000	20002443004	1
Sanacorp	Macrogol 4000	20003397011	1
Sanacorp	Macrogol 4000	20003397014	1
Sanacorp	Macrogol 4000	21003792004	1
Sanacorp	Macrogol 4000	22003814013	1
Sanacorp	Macrogol 4000	22004213005	1
Sanacorp	Macrogol 4000	2204213005	1
Sanacorp	Macrogol 4000	2207019-03	1
Sanacorp	Macrogol 4000	24000623005	1
Sanacorp	Macrogol 4000	2707018-01	2
Sanacorp	Macrogol 4000	F03-3694101	1
VDL	Macrogol 4000	16308906	1
WE:Sanacorp 19.10.20…	Macrogol 4000	15406301	2

- 233 754 spectra from 1515 *Apo-Ident* customers from a total of 48 675 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Macrogol 4000* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Macrogol 4000* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	690	0	152 272
Type B	0	1490	0	200 414
Type C	0	2309	4	233 751

The substance/substance group *Macrogol 4000* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1304 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5973 %)
Type C	100.0000 % (> 99.9009 %)	99.8271 % (> 99.6974 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20690	20690	0,00	63,01
20975	20975	0,00	81,90
21065	21886	13,58	66,73
21357	21886	7,20	60,51
21841	21841	0,00	70,13
21886	21886	0,00	58,23
21903	21903	0,00	75,67
22567	22567	0,00	59,17
22570	22570	0,00	72,95
23021	21886	6,86	63,67
23174	23174	0,00	74,90
23902	23902	0,00	78,71
25414	25414	0,00	77,29
25713	25713	0,00	78,33
26262	26262	0,00	76,70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Maleato de enalapril**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10003565-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Maleato de enalapril; Enalapril, maleato; Enalaprili maleas

Special notes

When selecting the *Maleato de enalapril* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Maleato de enalapril	6	3	12

Second-stage model

For differentiation of the substance/substance group *Maleato de enalapril* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Maleato de enalapril* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	102,68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Maleato de enalapril* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Maleato de enalapril*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Maleato de enalapril	16K14-B02-336220	23716	40	1801425
Fagron	Maleato de enalapril	17J18-B03-347278	24096	40	20171208
Fagron	Maleato de enalapril	20F26-F02-372725	25444	40	20200812
Fagron	Maleato de enalapril	22F29-B02-223143	26377	40	20220713
Fagron	Maleato de enalapril	22F29-B02-223143	26377SI	20	20220713
Fagron	Maleato de enalapril	23C23-B01-227968	26683	40	20230427
Fagron	Maleato de enalapril	23H22-B08-232432	27031	40	20230919

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 7 reference samples from the substance/substance group *Maleato de enalapril*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Maleato de enalapril*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Maleato de enalapril	19H27-F02-364744	24945	40
Fagron	Maleato de enalapril	21B19-F03-377278	25840	50
Fagron	Maleato de enalapril	21G22-B04-218923	26329	40
Fagron	Maleato de enalapril	21G22-B04-218923	26329SI	20
Fagron	Maleato de enalapril	23C23-B01-227968	26683SI†	20

- 201 914 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 28 *Apo-Ident* customers from 15 batches from the substance/substance group *Maleato de enalapril*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Maleato de enalapril	21G22-B04-218923	1
	Maleato de enalapril	23C23-B01-227968	2
Fagron	Maleato de enalapril	19H27-F02-364744	2
Fagron	Maleato de enalapril	1G22-B04-218923	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Maleato de enalapril	20F26-F02	1
Fagron	Maleato de enalapril	20F26-F02-372725	12
Fagron	Maleato de enalapril	21B19-F03-3772708	1
Fagron	Maleato de enalapril	21B19-F03-377278	5
Fagron	Maleato de enalapril	21G22-B04	2
Fagron	Maleato de enalapril	21G22-B04-218923	3
Fagron	Maleato de enalapril	22F29-B02-223143	1
Fagron	Maleato de enalapril	20F26-F02-372725	1
Fagron	Maleato de enalapril	3012-2004-008	1
Fagron	Maleato de enalapril	811-01000	1
Fagron	Maleato de enalapril	F02-3272005	1
Jenne	Maleato de enalapril	23C23-B01-227968	1
Nachprüfung	Maleato de enalapril	AP200615-11	1
Noweda	Maleato de enalapril	22F29-B02-223143	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 243 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Maleato de enalapril* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Maleato de enalapril* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	170	0	201 914
Type C	0	38	0	236 029

The substance/substance group *Maleato de enalapril* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.2105 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23716	23716	0,00	222,19
24096	23716	6,67	228,49
25444	23716	10,96	222,78
26377	23716	9,08	222,98
26683	23716	11,60	221,50
27031	23716	18,39	228,64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Maleato de feniramina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20694-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Maleato de feniramina; Feniramina, maleato; Pheniramini maleas

Special notes

When selecting the *Maleato de feniramina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Maleato de feniramina	6	5	41

Second-stage model

For differentiation of the substance/substance group *Maleato de feniramina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Maleato de feniramina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	74,35	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Maleato de feniramina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Maleato de feniramina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Maleato de feniramina	12200502	20694	40	1401559
Caelo	Maleato de feniramina	15172702	22790	40	1908273
Euro OTC	Maleato de feniramina	1910024	24921	40	20191122*
Euro OTC	Maleato de feniramina	2209021	26348	40	20221018*
Euro OTC	Maleato de feniramina	2209021	26348SI	20	20221018*
Fagron	Maleato de feniramina	13D24-N04	20928	40	20130530
Fagron	Maleato de feniramina	18C21-B02-362029	24948	40	20180426

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Maleato de feniramina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Maleato de feniramina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Maleato de feniramina	173167	23821	40
Euro OTC	Maleato de feniramina	1109013-02	20756	40
Euro OTC	Maleato de feniramina	1701021	23384	40
Euro OTC	Maleato de feniramina	2304009	26640	40
Fagron	Maleato de feniramina	23B02-B03-222367	26668	40
Euro OTC	Maleato de feniramina	2304009	26640SI	20
Fagron	Maleato de feniramina	23B02-B03-222367	26668SI	20

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 96 spectra from 48 *Apo-Ident* customers from 42 batches from the substance/substance group *Maleato de feniramina*.

- Among them are spectra of independent samples from 41 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Maleato de feniramina	2209021-01	1
Alliance Healthcare	Maleato de feniramina	12L04-N05	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Maleato de feniramina	17316706	2
Caelo	Maleato de feniramina	12352602	1
Caelo	Maleato de feniramina	12352604	1
Caelo	Maleato de feniramina	1235611	1
Caelo	Maleato de feniramina	14C25-B01-292540	1
Caelo	Maleato de feniramina	14C25-B01-302272	1
Caelo	Maleato de feniramina	14C25-B01-322989	1
Caelo	Maleato de feniramina	15172704	1
Caelo	Maleato de feniramina	15172708	1
Caelo	Maleato de feniramina	15172711	1
Caelo	Maleato de feniramina	173167001	1
Caelo	Maleato de feniramina	173167002	2
Caelo	Maleato de feniramina	173167003	1
Caelo	Maleato de feniramina	17316702	1
Caelo	Maleato de feniramina	17316705	1
Caelo	Maleato de feniramina	17316706	3
Caelo	Maleato de feniramina	17316707	1
Caelo	Maleato de feniramina	17316708	1
Caelo	Maleato de feniramina	9276210	1
Caesar & Loretz GmbH	Maleato de feniramina	173167002	6
Cealo	Maleato de feniramina	12352608	1
EuRO 14.11.2013 Phönix	Maleato de feniramina	1209032-01	1
Euro OTC	Maleato de feniramina	1109013-01	1
Euro OTC	Maleato de feniramina	1209032-01	2
Euro OTC	Maleato de feniramina	1411044-01	1
Euro OTC	Maleato de feniramina	1411044-02	3
Euro OTC	Maleato de feniramina	1701021-01	19
Euro OTC	Maleato de feniramina	1910024-01	1
Euro OTC	Maleato de feniramina	1910024-02	2
Euro OTC	Maleato de feniramina	2209021-01	2
Fagron	Maleato de feniramina	12I06-N02	1
Fagron	Maleato de feniramina	12L04-N05	3
Fagron	Maleato de feniramina	14C25-B01-292540	1
Fagron	Maleato de feniramina	14C25-B01-295293	3
Fagron	Maleato de feniramina	14c25b01307150	1
Fagron	Maleato de feniramina	14c25-b01-307150	1
Fagron	Maleato de feniramina	14C25-B01-307150	3
Fagron	Maleato de feniramina	14C25-B01-328732	2
Fagron	Maleato de feniramina	18C21-B02-351507	2
Fagron	Maleato de feniramina	18C21-B02-357417	1
Fagron	Maleato de feniramina	18C21-B02-369804	1
Fagron	Maleato de feniramina	18C21B02370926	1
Noweda 28.08.2019	Maleato de feniramina	15172714	1
Noweda	Maleato de feniramina	1701021	1
Sanacorp	Maleato de feniramina	18C21-B02-369804	1
Spangro_09.01.2019	Maleato de feniramina	1701021-01	7
Supriya LifeScience ...	Maleato de feniramina	SLL/P/1213063	1
Supriya LifeScience ...	Maleato de feniramina	14C25-B01	1

- 235 971 spectra from 1515 *Apo-Ident* customers from a total of 49 216 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Maleato de feniramina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

purpose, all relevant spectra of the various substances were compared with *Maleato de feniramina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	240	0	201 844
Type C	0	95	1	235 971

The substance/substance group *Maleato de feniramina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.9583 % (> 95.8333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20694	20694	0,00	181,96
20928	20694	13,56	175,45
22790	22790	0,00	175,47
24921	24921	0,00	174,64
24948	22790	23,31	170,01
26348	26348	0,00	174,02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Maltodextrina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20709-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Maltodextrina; Maltodextrinum

Special notes

When selecting the *Maltodextrina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Maltodextrina	2	1	3

Second-stage model

For differentiation of the substance/substance group *Maltodextrina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Maltodextrina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Amido de arroz	23,97	15,60
SyrSpend® SF pH4 neo	26,64	13,17
SyrSpend® SF pH4	32,86	20,56
Amido de trigo	33,68	17,24
Amido de milho	35,80	24,18
SyrSpend® SF Alka	41,62	18,57
Goma arábica, dispersão seca	54,36	30,27
⋮	⋮	⋮
Fécula de batata	>50	19,16
Carmelose sódica	>50	25,12
Sulfato de colistina	>50	30,09
Sulfato de polimixina B	>50	36,46
Glicerofosfato de cálcio	>50	44,23
Anfotericina B	>50	49,98
Bacitracina	>50	56,46
Riboflavina	>50	62,26
Cianocobalamina	>50	67,39
Tosilcloramida sódica	>50	77,62
Levedura de selênio	>50	78,34
Frutose	>50	83,56
Pantotenato de cálcio	>50	86,25
Nistatina	>50	90,48
Ácido oxálico	>50	105,58
Gelatina, branca	>50	108,39
Bromidrato de hioscina	>50	118,56
Estradiol hemi-hidratado	>50	125,62
Triancinolona	>50	136,33
Vitamina E acetato pó 50%	>50	142,86
Estriol	>50	175,56
Metilcobalamina	>50	186,75

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Maltodextrina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Maltodextrina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Gatt-Koller	Maltodextrina	21J01645	26382	40	20210909
Gatt-Koller	Maltodextrina	21J01645	26382SI	20	20210909
Inresa	Maltodextrina	R1503902	21806	60	AR-15-FG-008821-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Maltodextrina*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 842 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 1 reference samples from the substance/substance group *Maltodextrina*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Maltodextrina	R1600014	22314	60

- 202 024 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Maltodextrina*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
HBK Gesundheit	Maltodextrina	1143	3
HBK Gesundheit	Maltodextrina	2343	1
Phönix	Maltodextrina	LOT20250206JB	1

- 236 062 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Maltodextrina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Maltodextrina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	60	0	202 024
Type C	0	5	0	236 062

The substance/substance group *Maltodextrina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21806	21806	0,00	42,05
26382	21806	14,43	43,54

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Manitol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20118-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Manitol; Mannitolum

Special notes

When selecting the *Manitol* substance/substance group, the following information is displayed to the user:

- Observação: A presença e a ausência de sílica não são detectáveis no NIR. Verifique a densidade aparente, se necessário.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Manitol	8	36	870

Second-stage model

For differentiation of the substance/substance group *Manitol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Manitol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	81,59	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Manitol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Manitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Manitol	12305723	20980	40	1402329
Caelo	Manitol	15197305	22581	40	20150720
Euro OTC	Manitol	1508012	21884	60	20150827*
Euro OTC	Manitol	1511025	22286	60	20151228*
Euro OTC	Manitol	2011022	25548	40	20210112*
Fagron	Manitol	15A26-B01-305841	22883	40	20150204
Fagron	Manitol	15A26-B01-305841	22884	40	20150204
Fagron	Manitol	17B08-B04-352402	24579	40	20170517
Fagron	Manitol	22D25-B04-224320	26396	40	20220629
Fagron	Manitol	22D25-B04-224320	26396SI	20	20220629

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Manitol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1670 spectra of 43 reference samples from the substance/substance group *Manitol*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Manitol	160140	22458	60
Caelo	Manitol	16014013	22580	40
Caelo	Manitol	162009	22614	40
Caelo	Manitol	162121	22721	40
Caelo	Manitol	170879	23296	40
Caelo	Manitol	170450	23318	40
Caelo	Manitol	172588	23800	40
Caelo	Manitol	182654	24368	40
Caelo	Manitol	182655	24385	40
Caelo	Manitol	191654	24723	40
Caelo	Manitol	22001495	26249	40
Caelo	Manitol	24000339	27137	40
Euro OTC	Manitol	1604008	22515	40
Euro OTC	Manitol	1606031	22697	40
Euro OTC	Manitol	1610027	22862	40
Euro OTC	Manitol	1703043	23125	40
Euro OTC	Manitol	1708005	23700	40
Euro OTC	Manitol	1802004	23966	40
Euro OTC	Manitol	1806024	24152	40
Euro OTC	Manitol	1809008	24327	40
Euro OTC	Manitol	1902011	24476	40
Euro OTC	Manitol	1904025	24600	40
Euro OTC	Manitol	1908019	24857	40
Euro OTC	Manitol	2004015	25161	40
Euro OTC	Manitol	2008030	25323	40
Euro OTC	Manitol	2105014	25678	40
Euro OTC	Manitol	2108016	25822	50
Euro OTC	Manitol	2108015	25826	50
Euro OTC	Manitol	2108014	25828	50

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Manitol	2201036	25957	40
Euro OTC	Manitol	2205036	26218	40
Euro OTC	Manitol	2209020	26343	40
Euro OTC	Manitol	2301038	26598	40
Euro OTC	Manitol	2307004	26858	40
Euro OTC	Manitol	2401022	27149	40
Fagron	Manitol	18H16-B01	24817	40
Caelo	Manitol	162121	23066	30
Caelo	Manitol	160140	23299	40
Caelo	Manitol	170879	23305	40
Caelo	Manitol	22001495	26249SI	20
Euro OTC	Manitol	2201036	25957SI	10
Euro OTC	Manitol	2205036	26218SI	20
Euro OTC	Manitol	2209020	26343SI	20

- 200 414 spectra from a total of 4009 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3271 spectra from 824 *Apo-Ident* customers from 877 batches from the substance/substance group *Manitol*.
- Among them are spectra of independent samples from 868 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Manitol	20003605012	1
	Manitol	21000744042	1
	Manitol	21K16-B11-216336	2
	Manitol	22001495005	2
	Manitol	22001495015	7
	Manitol	22001495017	3
	Manitol	22001495019	1
	Manitol	22001495023	3
	Manitol	22001495041	1
	Manitol	22001495046	1
	Manitol	22001712003	1
	Manitol	22001712004	2
	Manitol	22001712008	5
	Manitol	22001712009	1
	Manitol	22001712010	1
	Manitol	22001712011	7
	Manitol	22001712012	2
	Manitol	2201036-01	2
	Manitol	2201495041	1
	Manitol	2205036-01	3
	Manitol	2209020-01	3
	Manitol	22B22-F09	1
	Manitol	22D25-B04-233814	1
	Manitol	22E23-F15-38121	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Manitol	22F15-F10-382723	1
	Manitol	22F15-F15	2
	Manitol	22F15-F20-382742	1
	Manitol	2301038-01	2
	Manitol	2307004-01	8
	Manitol	2312007-01	2
	Manitol	23A10-F03-384081	1
	Manitol	23A10-F09	1
	Manitol	23A10-F09-384083	1
	Manitol	23A24F02-384302	1
	Manitol	23A24-F02-384302	2
	Manitol	23A24-F03-284303	1
	Manitol	23A24-F03-38303	1
	Manitol	23A24-F03-384303	2
	Manitol	23A24-F05-384305	3
	Manitol	23A24-F06-384306	1
	Manitol	23A24-F07-384307	1
	Manitol	23A24-F15-384487	2
	Manitol	24000339007	4
	Manitol	24000356001	2
	Manitol	24000356002	3
	Manitol	24000356003	3
	Manitol	24000356005	1
	Manitol	24000356007	2
	Manitol	24000356010	1
AHC	Manitol	18265511	1
AHC	Manitol	20000958003	1
AHC	Manitol	23I01-F01	1
AHD/EuRho02	Manitol	1904025-02	1
AHD	Manitol	2200195015	1
AHD	Manitol	23A24-F04-384304	1
AHD	Manitol	23A24-F05-384305	1
ALH/EuRho	Manitol	1802004-01	1
ALH	Manitol	1409016-01	1
ALH	Manitol	1703043-01	1
Alliance / Fargon	Manitol	19B12-B02-359604	1
Alliance Health 12.0...	Manitol	1404034-01	2
Alliance Healthcare	Manitol	18265409	1
Alliance Healthcare	Manitol	2004015-01	1
alliance	Manitol	2307004-01	1
Allianz Healthcare 2...	Manitol	1502022-01	1
allianz	Manitol	16212101	2
Anzag 05.10.17 8,04EUR	Manitol	17045002	1
ANZAG	Manitol	1211034-01	1
Anzag	Manitol	1310004-02	1
Anzag	Manitol	20003605007	3
Apo Ident/ Noweda	Manitol	1610027-01	1
ApoIdent/Noweda	Manitol	1610027-01	1
apomix	Manitol	1310004-01	1
apomix	Manitol	1708005-01	2
Bombastus	Manitol	16340301	1
Cael Sanacorp 05.02.2016	Manitol	14323138	2
Caeleo/ Kehr	Manitol	182654001	1
Caelo	Manitol		1
Caelo	Manitol	10011501	1
Caelo	Manitol	10100026	2
Caelo	Manitol	1071701	1
Caelo	Manitol	11(16200912)	1
Caelo	Manitol	11003611	1
Caelo	Manitol	1110009-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manitol	11219121	1
Caelo	Manitol	11219122	1
Caelo	Manitol	11219124	2
Caelo	Manitol	11308807	2
Caelo	Manitol	11D01-N10	1
Caelo	Manitol	1205016-01	2
Caelo	Manitol	1205016-02	2
Caelo	Manitol	12105403	3
Caelo	Manitol	12105404	3
Caelo	Manitol	12105405	1
Caelo	Manitol	12105420	7
Caelo	Manitol	12105421	9
Caelo	Manitol	12105433	6
Caelo	Manitol	12105438	2
Caelo	Manitol	1211034-01	1
Caelo	Manitol	12305709	16
Caelo	Manitol	12305710	8
Caelo	Manitol	12305723	4
Caelo	Manitol	12305724	5
Caelo	Manitol	12305725	11
Caelo	Manitol	12305725-3444311112	1
Caelo	Manitol	12305726	1
Caelo	Manitol	12305728	2
Caelo	Manitol	12305734	2
Caelo	Manitol	12305736	4
Caelo	Manitol	12305740	2
Caelo	Manitol	1230578	1
Caelo	Manitol	12411754	1
Caelo	Manitol	1305043-02	3
Caelo	Manitol	13095013	1
Caelo	Manitol	1310004-01	3
Caelo	Manitol	13189201	8
Caelo	Manitol	13189203	8
Caelo	Manitol	13189203-3566412081	1
Caelo	Manitol	13189206	1
Caelo	Manitol	13189207	8
Caelo	Manitol	13189208	6
Caelo	Manitol	13189215	17
Caelo	Manitol	13189222	3
Caelo	Manitol	13189226	4
Caelo	Manitol	13189227	11
Caelo	Manitol	13189228	1
Caelo	Manitol	13K20-B01-287704	1
Caelo	Manitol	14(20000685001)	1
Caelo	Manitol	1400434-01	1
Caelo	Manitol	1404034-01	2
Caelo	Manitol	14051204	8
Caelo	Manitol	14051205	7
Caelo	Manitol	14051207	1
Caelo	Manitol	14051208	2
Caelo	Manitol	14051209	7
Caelo	Manitol	14051215	7
Caelo	Manitol	14051216	3
Caelo	Manitol	14051217	2
Caelo	Manitol	14051223	1
Caelo	Manitol	14051224	2
Caelo	Manitol	14051229	6
Caelo	Manitol	14051230	2
Caelo	Manitol	1405127	1
Caelo	Manitol	1409016-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manitol	1423120	1
Caelo	Manitol	14323101	3
Caelo	Manitol	14323103	3
Caelo	Manitol	14323105	2
Caelo	Manitol	14323113	1
Caelo	Manitol	14323114	3
Caelo	Manitol	14323115	4
Caelo	Manitol	14323120	1
Caelo	Manitol	14323121	6
Caelo	Manitol	14323124	2
Caelo	Manitol	14323125	2
Caelo	Manitol	14323126	4
Caelo	Manitol	14323127	5
Caelo	Manitol	14323129	1
Caelo	Manitol	14323138	24
Caelo	Manitol	14G04-B07-301693	2
Caelo	Manitol	14g04-b07-30692	1
Caelo	Manitol	1502022-01	1
Caelo	Manitol	1508012-01	2
Caelo	Manitol	1508012-02	1
Caelo	Manitol	1511025-01	1
Caelo	Manitol	151117	1
Caelo	Manitol	15184101	1
Caelo	Manitol	1519713	1
Caelo	Manitol	15197219	1
Caelo	Manitol	15197301	14
Caelo	Manitol	15197302	5
Caelo	Manitol	15197303	1
Caelo	Manitol	15197312	1
Caelo	Manitol	15197313	17
Caelo	Manitol	15197314	6
Caelo	Manitol	15197319	8
Caelo	Manitol	15197327	1
Caelo	Manitol	15197329	1
Caelo	Manitol	15525	1
Caelo	Manitol	15D28-B02-309192	4
Caelo	Manitol	15K25-B04	1
Caelo	Manitol	16011402	1
Caelo	Manitol	16014005	12
Caelo	Manitol	16014013	1
Caelo	Manitol	16014014	1
Caelo	Manitol	16014016	1
Caelo	Manitol	160400801	2
Caelo	Manitol	1606031-02	1
Caelo	Manitol	16061401	1
Caelo	Manitol	1610018-01	1
Caelo	Manitol	1610027-01	3
Caelo	Manitol	1612101	1
Caelo	Manitol	16200901	2
Caelo	Manitol	16200903	14
Caelo	Manitol	16200904	2
Caelo	Manitol	16200908	2
Caelo	Manitol	16200909	1
Caelo	Manitol	16200912	5
Caelo	Manitol	16200913	4
Caelo	Manitol	16200916	2
Caelo	Manitol	16200924	11
Caelo	Manitol	162121	1
Caelo	Manitol	16212101	14
Caelo	Manitol	16212102	15

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manitol	16212103	1
Caelo	Manitol	16212104	2
Caelo	Manitol	16212106	4
Caelo	Manitol	16212109	4
Caelo	Manitol	1621212	1
Caelo	Manitol	16236603	1
Caelo	Manitol	163403	1
Caelo	Manitol	16340301	16
Caelo	Manitol	16340302	7
Caelo	Manitol	16D20-B03	1
Caelo	Manitol	16F27-B05-324516	1
Caelo	Manitol	16G27-B03	1
Caelo	Manitol	16H25-B03-326639	1
Caelo	Manitol	16H29-B05-327813	1
Caelo	Manitol	16L15-B04-329317	1
Caelo	Manitol	17/13-B03-340967	1
Caelo	Manitol	17/13-B11	1
Caelo	Manitol	1703043-01	1
Caelo	Manitol	170450	1
Caelo	Manitol	17045001	4
Caelo	Manitol	17045002	19
Caelo	Manitol	17045003	9
Caelo	Manitol	17045004	3
Caelo	Manitol	17045006	2
Caelo	Manitol	17045008	7
Caelo	Manitol	17045009	19
Caelo	Manitol	17045010	5
Caelo	Manitol	17050032/3	1
Caelo	Manitol	170800501	3
Caelo	Manitol	1708005-01	1
Caelo	Manitol	17087907	1
Caelo	Manitol	17087908	9
Caelo	Manitol	17087909	3
Caelo	Manitol	17087915	2
Caelo	Manitol	17087916	21
Caelo	Manitol	17258808	5
Caelo	Manitol	17258809	11
Caelo	Manitol	17258812	7
Caelo	Manitol	17258819	5
Caelo	Manitol	17258820	7
Caelo	Manitol	17258823	3
Caelo	Manitol	17258830	4
Caelo	Manitol	17258830/P-09041922	1
Caelo	Manitol	17258830/P-23051923	1
Caelo	Manitol	17258831	4
Caelo	Manitol	17260101	1
Caelo	Manitol	17360101	20
Caelo	Manitol	17360108	22
Caelo	Manitol	17360110	5
Caelo	Manitol	17360112	11
Caelo	Manitol	17360114	1
Caelo	Manitol	17360115	8
Caelo	Manitol	17A12-B03	1
Caelo	Manitol	17I13-B02-340966	1
Caelo	Manitol	17j23-B05	1
Caelo	Manitol	17J30B09343413	1
Caelo	Manitol	17J30-B10-3434414	1
Caelo	Manitol	17K29-B07-344253	1
Caelo	Manitol	1802004-01	2
Caelo	Manitol	180602401	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manitol	1806024-01	2
Caelo	Manitol	1809008-01	3
Caelo	Manitol	18121701	1
Caelo	Manitol	1826504001	1
Caelo	Manitol	182654001	1
Caelo	Manitol	18265409	1
Caelo	Manitol	18265410	5
Caelo	Manitol	18265411	7
Caelo	Manitol	18265417	3
Caelo	Manitol	18265418	3
Caelo	Manitol	18265427	1
Caelo	Manitol	18265428	2
Caelo	Manitol	18265429	1
Caelo	Manitol	18265432	3
Caelo	Manitol	18265436	2
Caelo	Manitol	182655001	15
Caelo	Manitol	182655002	1
Caelo	Manitol	182655004	10
Caelo	Manitol	18265502	15
Caelo	Manitol	18265503	1
Caelo	Manitol	18265504	5
Caelo	Manitol	18265505	1
Caelo	Manitol	18265506	17
Caelo	Manitol	18265507	7
Caelo	Manitol	18265508	11
Caelo	Manitol	18265509	6
Caelo	Manitol	18265511	12
Caelo	Manitol	18265512	11
Caelo	Manitol	18266513	1
Caelo	Manitol	18A30-B03-346849	1
Caelo	Manitol	18A30-B08	1
Caelo	Manitol	18b23-b09	1
Caelo	Manitol	18D09-B11-351436	1
Caelo	Manitol	18D09-B12-351437	3
Caelo	Manitol	18D09-B13-352214	2
Caelo	Manitol	18D09-B14-352215	1
Caelo	Manitol	18D09-B16-252503	1
Caelo	Manitol	18e25-b07-352753	1
Caelo	Manitol	19120-F15	1
Caelo	Manitol	191654002	1
Caelo	Manitol	191654003	2
Caelo	Manitol	191654004	1
Caelo	Manitol	19165401	6
Caelo	Manitol	191654011	3
Caelo	Manitol	191654012	1
Caelo	Manitol	19165402	3
Caelo	Manitol	19165403	1
Caelo	Manitol	19165407	2
Caelo	Manitol	19654002	1
Caelo	Manitol	19J09-F07-366954	2
Caelo	Manitol	19L19F14366950	1
Caelo	Manitol	20000068507	1
Caelo	Manitol	2000058001	1
Caelo	Manitol	20000685001	7
Caelo	Manitol	20000685006	2
Caelo	Manitol	20000685007	2
Caelo	Manitol	20000685008	1
Caelo	Manitol	20000685012	15
Caelo	Manitol	20000685013	3
Caelo	Manitol	20000685014	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manitol	20000685017	1
Caelo	Manitol	20000685021	1
Caelo	Manitol	20000958001	11
Caelo	Manitol	20000958003	7
Caelo	Manitol	20000958006	7
Caelo	Manitol	20000958007	6
Caelo	Manitol	20001038003	1
Caelo	Manitol	20002605010	1
Caelo	Manitol	20003601002	1
Caelo	Manitol	20003605002	8
Caelo	Manitol	20003605003	1
Caelo	Manitol	20003605004	12
Caelo	Manitol	20003605006	1
Caelo	Manitol	20003605007	11
Caelo	Manitol	20003605008	5
Caelo	Manitol	20003605010	9
Caelo	Manitol	20003605011	2
Caelo	Manitol	20003605013	9
Caelo	Manitol	20003605015	5
Caelo	Manitol	2000360510	2
Caelo	Manitol	20003605504	1
Caelo	Manitol	20004038002	1
Caelo	Manitol	20004038003	5
Caelo	Manitol	20004038004	2
Caelo	Manitol	20004038006	1
Caelo	Manitol	20004038007	5
Caelo	Manitol	2000685006	1
Caelo	Manitol	2000685014	1
Caelo	Manitol	2000958003	1
Caelo	Manitol	200218P302	1
Caelo	Manitol	2003605007	1
Caelo	Manitol	20151012-2	1
Caelo	Manitol	20B05-F04-369845	1
Caelo	Manitol	20H21F05373849	1
Caelo	Manitol	21000744014	2
Caelo	Manitol	21000744015	4
Caelo	Manitol	21000744021	1
Caelo	Manitol	21000744029	1
Caelo	Manitol	21000744033	1
Caelo	Manitol	21000744042	1
Caelo	Manitol	2100074412	1
Caelo	Manitol	2100074414	1
Caelo	Manitol	2100342002	1
Caelo	Manitol	21003432001	5
Caelo	Manitol	21003432002	8
Caelo	Manitol	2101401	1
Caelo	Manitol	210501401	1
Caelo	Manitol	2105014-01	1
Caelo	Manitol	22001495002	2
Caelo	Manitol	22001495009	1
Caelo	Manitol	2200149501	1
Caelo	Manitol	22001495016	2
Caelo	Manitol	22001495017	1
Caelo	Manitol	22001712001	2
Caelo	Manitol	22001712003	3
Caelo	Manitol	22001712004	3
Caelo	Manitol	22001712007	1
Caelo	Manitol	2274635	1
Caelo	Manitol	23082013C	1
Caelo	Manitol	24101306	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manitol	27101802	1
Caelo	Manitol	30031502	1
Caelo	Manitol	30121417	1
Caelo	Manitol	4414E-01844	1
Caelo	Manitol	4516E-01844	1
Caelo	Manitol	48558	1
Caelo	Manitol	5031304	1
Caelo	Manitol	514E-01844	1
Caelo	Manitol	7071404	1
Caelo	Manitol	8031704	1
Caelo	Manitol	8720	1
Caelo	Manitol	9061808	1
Caelo	Manitol	9081303	1
Caelo	Manitol	9204719	1
Caelo	Manitol	E911K	1
Caelo	Manitol	E976E	1
Caesar & Lorenz GmbH	Manitol	18265507	1
Caesar & Loretz GmbH…	Manitol	16200908	1
Caesar & Loretz GmbH…	Manitol	18265509	1
Caesar & Loretz GmbH…	Manitol	21000744006	1
Caesar & Loretz GmbH…	Manitol	17258819	1
Caesar & Loretz GmbH/AHD	Manitol	20003605011	1
Caesar & Loretz GmbH/GEHE	Manitol	182655001	1
Caesar & Loretz GmbH/GEHE	Manitol	20000958003	1
Caesar & Loretz GmbH/GEHE	Manitol	20000958007	1
Caesar & Loretz GmbH/GEHE	Manitol	20003605002	2
Caesar & Loretz GmbH…	Manitol	191654004	1
Caesar & Loretz GmbH…	Manitol	20000685007	4
Caesar & Loretz GmbH…	Manitol	20004038004	2
Caesar & Loretz GmbH…	Manitol	18265509	1
Caesar & Loretz GmbH…	Manitol	18265512	1
Caesar & Loretz GmbH/Kehr	Manitol	182655001	1
Caesar & Loretz GmbH/Kehr	Manitol	18265508	1
Caesar & Loretz GmbH…	Manitol	18265432	3
Caesar & Loretz GmbH…	Manitol	17258809	1
Caesar & Loretz GmbH…	Manitol	18265511	2
Caesar & Loretz GmbH/Phö	Manitol	20000958003	1
Caesar & Loretz GmbH/Phoe	Manitol	20003605007	1
Caesar & Loretz GmbH…	Manitol	20003605012	1
Caesar & Loretz GmbH…	Manitol	22001712004	14
Caesar & Loretz GmbH…	Manitol	20000685014	1
Caesar & Loretz GmbH…	Manitol	20003605002	1
Caesar & Loretz GmbH/Sana	Manitol	20003605002	1
Caesar & Loretz GmbH…	Manitol	2000058001	1
Caesar & Loretz GmbH	Manitol	13189207	1
Caesar & Loretz GmbH	Manitol	14323119	1
Caesar & Loretz GmbH	Manitol	17087915	1
Caesar & Loretz GmbH	Manitol	17258809	2
Caesar & Loretz GmbH	Manitol	17258819	1
Caesar & Loretz GmbH	Manitol	17258820	1
Caesar & Loretz GmbH	Manitol	17360112	1
Caesar & Loretz GmbH	Manitol	17360114	2
Caesar & Loretz GmbH	Manitol	1826508	1
Caesar & Loretz GmbH	Manitol	18265408	2
Caesar & Loretz GmbH	Manitol	18265409	1
Caesar & Loretz GmbH	Manitol	18265417	3
Caesar & Loretz GmbH	Manitol	18265418	2
Caesar & Loretz GmbH	Manitol	18265420	5
Caesar & Loretz GmbH	Manitol	18265431	1
Caesar & Loretz GmbH	Manitol	182655001	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Manitol	182655002	5
Caesar & Loretz GmbH	Manitol	182655004	2
Caesar & Loretz GmbH	Manitol	18265502	3
Caesar & Loretz GmbH	Manitol	18265503	2
Caesar & Loretz GmbH	Manitol	18265504	7
Caesar & Loretz GmbH	Manitol	18265505	4
Caesar & Loretz GmbH	Manitol	18265506	3
Caesar & Loretz GmbH	Manitol	18265507	1
Caesar & Loretz GmbH	Manitol	18265508	10
Caesar & Loretz GmbH	Manitol	18265509	1
Caesar & Loretz GmbH	Manitol	18265510	1
Caesar & Loretz GmbH	Manitol	18265511	4
Caesar & Loretz GmbH	Manitol	18265512	2
Caesar & Loretz GmbH	Manitol	191654004	3
Caesar & Loretz GmbH	Manitol	19165401	3
Caesar & Loretz GmbH	Manitol	191654012	1
Caesar & Loretz GmbH	Manitol	20000685001	3
Caesar & Loretz GmbH	Manitol	20000685007	1
Caesar & Loretz GmbH	Manitol	20000958001	5
Caesar & Loretz GmbH	Manitol	20000958003	2
Caesar & Loretz GmbH	Manitol	20000958006	1
Caesar & Loretz GmbH	Manitol	20000958007	6
Caesar & Loretz GmbH	Manitol	20003605002	3
Caesar & Loretz GmbH	Manitol	20003605004	3
Caesar & Loretz GmbH	Manitol	20003605006	1
Caesar & Loretz GmbH	Manitol	20003605007	2
Caesar & Loretz GmbH	Manitol	20003605008	1
Caesar & Loretz GmbH	Manitol	20003605010	2
Caesar & Loretz GmbH	Manitol	20003605012	2
Caesar & Loretz GmbH	Manitol	20003605013	2
Caesar & Loretz GmbH	Manitol	20004038004	3
Caesar & Loretz GmbH	Manitol	21000744014	2
Caesar & Loretz GmbH	Manitol	21000744029	4
Caesar & Loretz GmbH	Manitol	21000744042	2
Caesar & Loretz GmbH	Manitol	21003432001	2
Caesar & Loretz GmbH	Manitol	21003432002	2
Caesar & Loretz GmbH	Manitol	22001495002	1
Caesar & Loretz GmbH	Manitol	22001495006	5
Caesar & Loretz GmbH	Manitol	22001495017	1
Caesar & Loretz GmbH	Manitol	22001712001	1
Caesar & Loretz GmbH	Manitol	22001712003	1
Caesar & Loretz GmbH	Manitol	22001712004	4
Caesar & Loretz GmbH	Manitol	22001712006	1
Caesar & Loretz GmbH	Manitol	22001712007	1
Caesar & Loretz/Noweda	Manitol	182655004	1
Caesar & Loretz/Noweda	Manitol	20003605004	1
Caesar & Loretz/Noweda	Manitol	20003605007	1
Caesar/Ebert	Manitol	17360108	1
Caesar	Manitol	1508012-1	1
Caleo/ Noweda	Manitol	18J04-B05-355467	1
Calo/Noweda	Manitol	23A10-F13-384084	1
ceal	Manitol	17045006	1
Cealo, Noweda	Manitol	20003605002	1
Cealo/Gehe	Manitol	18265502	1
cealo/phoenix	Manitol	14323138	2
Celo/Phoenix	Manitol	20003605004	1
Celo	Manitol	15197313	1
cesar&lorentz/Phönix	Manitol	12305710	1
Defektur/eigen	Manitol	1604008-01	1
Delta	Manitol	1610027-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Ebert & Jacobi	Manitol	12305728	1
EuRho Pharma	Manitol	1704010-01	1
EuRho/GEHE	Manitol	1409016-01	1
EuRho/GEHE	Manitol	1409016-02	1
EuRho/Gehe	Manitol	1802004-01	1
EuRho/Noweda	Manitol	1703043-01	1
EuRho/Noweda	Manitol	1806024-01	1
EuRho/Noweda	Manitol	1904025-01	2
EuRho/Phoenix	Manitol	1508012-01	1
EuRho/Sanac	Manitol	1305043-01	1
EuRho	Manitol	1205016-01	1
EuRho	Manitol	1211034-01	1
EuRho	Manitol	1211034-02	1
EuRho	Manitol	1404034-01	1
EuRho	Manitol	1404034-02	2
EuRho	Manitol	1502022-02	1
EuRho	Manitol	1508012-01	7
EuRho	Manitol	1511025-01	1
EuRho	Manitol	1911M-01844	1
EuRho	Manitol	2108016-01	1
Eurho	Manitol	2201036-01	2
EuRhoPha	Manitol	1404034-01	1
Euro OTC	Manitol	1006019-01	1
Euro OTC	Manitol	10112014E	1
Euro OTC	Manitol	1104028-01	1
Euro OTC	Manitol	1104028-03	3
Euro OTC	Manitol	1110009-01	10
Euro OTC	Manitol	1110009-02	4
Euro OTC	Manitol	111100009-02	1
Euro OTC	Manitol	1205016	1
Euro OTC	Manitol	1205016-01	11
Euro OTC	Manitol	1205016-02	2
Euro OTC	Manitol	12105433	3
Euro OTC	Manitol	1211034-01	9
Euro OTC	Manitol	1211034-02	14
Euro OTC	Manitol	1305043	1
Euro OTC	Manitol	130504301	1
Euro OTC	Manitol	1305043-01	12
Euro OTC	Manitol	1305043-02	14
Euro OTC	Manitol	1310004-01	14
Euro OTC	Manitol	1310004-02	8
Euro OTC	Manitol	13155710	1
Euro OTC	Manitol	13189216	2
Euro OTC	Manitol	14003402	1
Euro OTC	Manitol	140403401	1
Euro OTC	Manitol	1404034-01	15
Euro OTC	Manitol	140403402	2
Euro OTC	Manitol	1404034-02	16
Euro OTC	Manitol	1404036-02	1
Euro OTC	Manitol	1409016-01	19
Euro OTC	Manitol	1409016-02	6
Euro OTC	Manitol	1409016-1	1
Euro OTC	Manitol	15002022-01	1
Euro OTC	Manitol	1502022/01	1
Euro OTC	Manitol	150202201	2
Euro OTC	Manitol	1502022-01	17
Euro OTC	Manitol	150202202	1
Euro OTC	Manitol	1502022-02	5
Euro OTC	Manitol	150801	1
Euro OTC	Manitol	150801201	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Manitol	1508012-01	33
Euro OTC	Manitol	1508012-02	14
Euro OTC	Manitol	150916M	1
Euro OTC	Manitol	1511024-01	1
Euro OTC	Manitol	151102501	2
Euro OTC	Manitol	1511025-01	42
Euro OTC	Manitol	151105-01	1
Euro OTC	Manitol	158012-01	1
Euro OTC	Manitol	160027-01	1
Euro OTC	Manitol	16006031-01	1
Euro OTC	Manitol	160400	2
Euro OTC	Manitol	16040008-01	1
Euro OTC	Manitol	1604002-01	1
Euro OTC	Manitol	1604008	1
Euro OTC	Manitol	160400801	1
Euro OTC	Manitol	1604008-01	44
Euro OTC	Manitol	160408-01	1
Euro OTC	Manitol	160601-01	1
Euro OTC	Manitol	160603101	1
Euro OTC	Manitol	1606031-01	24
Euro OTC	Manitol	1606031-02	8
Euro OTC	Manitol	161002701	3
Euro OTC	Manitol	1610027-01	34
Euro OTC	Manitol	1610027-02	2
Euro OTC	Manitol	1610027-1	1
Euro OTC	Manitol	161129M/1604008-01	1
Euro OTC	Manitol	16D20-B04-320487	1
Euro OTC	Manitol	16H29-B02	1
Euro OTC	Manitol	17/14	1
Euro OTC	Manitol	170304301	3
Euro OTC	Manitol	1703043-01	16
Euro OTC	Manitol	170304302	1
Euro OTC	Manitol	1703043-02	11
Euro OTC	Manitol	1703049-01	1
Euro OTC	Manitol	1704010-01	6
Euro OTC	Manitol	1704010-10	1
Euro OTC	Manitol	1708005	1
Euro OTC	Manitol	170800501	1
Euro OTC	Manitol	1708005-01	42
Euro OTC	Manitol	1708005-02	4
Euro OTC	Manitol	1708005-05	1
Euro OTC	Manitol	17087908	1
Euro OTC	Manitol	178005-01	1
Euro OTC	Manitol	180200401	2
Euro OTC	Manitol	1802004-01	30
Euro OTC	Manitol	180219M/1708005-01	1
Euro OTC	Manitol	1806024/01	1
Euro OTC	Manitol	180602401	1
Euro OTC	Manitol	1806024-01	22
Euro OTC	Manitol	1806024-1	1
Euro OTC	Manitol	180624-01	2
Euro OTC	Manitol	1809008-001	1
Euro OTC	Manitol	1809008-002	1
Euro OTC	Manitol	1809008-01	32
Euro OTC	Manitol	180900802	1
Euro OTC	Manitol	1809008-02	19
Euro OTC	Manitol	1901092	2
Euro OTC	Manitol	1902011-01	20
Euro OTC	Manitol	1904023-03	1
Euro OTC	Manitol	1904025	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Manitol	190402501	1
Euro OTC	Manitol	1904025-01	16
Euro OTC	Manitol	190402502	1
Euro OTC	Manitol	1904025-02	44
Euro OTC	Manitol	1904025-03	19
Euro OTC	Manitol	1904025-12	1
Euro OTC	Manitol	190801901	1
Euro OTC	Manitol	1908019-01	1
Euro OTC	Manitol	1908019-02	5
Euro OTC	Manitol	19I20-F12	1
Euro OTC	Manitol	200401501	1
Euro OTC	Manitol	2004015-01	32
Euro OTC	Manitol	200803001	1
Euro OTC	Manitol	2008030-01	32
Euro OTC	Manitol	2011022-01	16
Euro OTC	Manitol	2011022-011	1
Euro OTC	Manitol	204015-01	1
Euro OTC	Manitol	20B05-F03-369844	1
Euro OTC	Manitol	2105014-01	15
Euro OTC	Manitol	2108014-01	4
Euro OTC	Manitol	2108015-01	6
Euro OTC	Manitol	2108016-01	5
Euro OTC	Manitol	2201036_01	1
Euro OTC	Manitol	2201036-01	11
Euro OTC	Manitol	2205036	1
Euro OTC	Manitol	2205036-01	7
Euro OTC	Manitol	2209020-01	9
Euro OTC	Manitol	2301038-01	2
Euro OTC	Manitol	E112N	2
Euro OTC	Manitol	e118t	1
Euro OTC	Manitol	E118T	3
Euro OTC	Manitol	E224X	1
Euro OTC	Manitol	E235L	1
Euro OTC	Manitol	E312J	1
Euro OTC	Manitol	E331X	1
Euro OTC	Manitol	E671Z	1
Euro OTC	Manitol	E976E	2
Euro OTC	Manitol	T03-07/1409016-01	1
Euro/Gehe	Manitol	1508012-01	2
Euro/Noweda	Manitol	1902011-01	2
Euro/Phönix	Manitol	1904025-02	1
EURO	Manitol	170401001	1
EurpTec/ Alliance He...	Manitol	1610027-02	1
Fagon	Manitol	13K20-B01-292064	1
Fagron	Manitol		1
Fagron	Manitol	10974140	1
Fagron	Manitol	11219122	1
Fagron	Manitol	11L19-N15	1
Fagron	Manitol	12E24-N03	1
Fagron	Manitol	12J26-N15	1
Fagron	Manitol	12K28-N01	1
Fagron	Manitol	1302C004	2
Fagron	Manitol	1302C005	1
Fagron	Manitol	13B01-B05-283812	1
Fagron	Manitol	13E24N01	1
Fagron	Manitol	13K20-B01	1
Fagron	Manitol	13K20-B01-287698	2
Fagron	Manitol	13K20-B01-287706	1
Fagron	Manitol	13K20-B01-294193	1
Fagron	Manitol	13K20-B01-294194	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Manitol	14323121	1
Fagron	Manitol	14G004-B07-301692	1
Fagron	Manitol	14G04-B07	4
Fagron	Manitol	14G04-B07-296196	1
Fagron	Manitol	14G04-B07-301685	1
Fagron	Manitol	14G04-B07-301692	15
Fagron	Manitol	14G04-B07-301693	1
Fagron	Manitol	14G04-B07-301694	1
Fagron	Manitol	14G17-B06-301921	1
Fagron	Manitol	1502022-01	3
Fagron	Manitol	15A26-B01-304717	4
Fagron	Manitol	15B05-B04-304084	4
Fagron	Manitol	15B05-B05-304085	1
Fagron	Manitol	15C04-B04-311796	1
Fagron	Manitol	15D28-B02-309192	4
Fagron	Manitol	15D28-B02-309193	1
Fagron	Manitol	15I24-B04	1
Fagron	Manitol	15K17-B01-315560	3
Fagron	Manitol	15K17-B03-314903	1
Fagron	Manitol	15K25-B04-317786	2
Fagron	Manitol	15K25-B06-318740	3
Fagron	Manitol	16/28-B01-328593	1
Fagron	Manitol	16212103	1
Fagron	Manitol	16340301	1
Fagron	Manitol	16B24-B09-32001	1
Fagron	Manitol	16B24-B09-320013	2
Fagron	Manitol	16D20-B03	1
Fagron	Manitol	16D20-B03-320486	1
Fagron	Manitol	16D20-B04-320487	1
Fagron	Manitol	16E11-B04	1
Fagron	Manitol	16E11-B06	1
Fagron	Manitol	16E11B07322830	1
Fagron	Manitol	16E11-B07-322830	2
Fagron	Manitol	16E11-B08	1
Fagron	Manitol	16E11-B08-323540	1
Fagron	Manitol	16F01-B03-322189	1
Fagron	Manitol	16F27-B04-32483	1
Fagron	Manitol	16F27-B05-324516	2
Fagron	Manitol	16G27-B03	1
Fagron	Manitol	16G27-B03-324517	1
Fagron	Manitol	16G27-B05-325659	2
Fagron	Manitol	16H02-B01-325660	1
Fagron	Manitol	16H25-B03-326639	3
Fagron	Manitol	16H29-B02-326640	2
Fagron	Manitol	16H29-B03-326641	1
Fagron	Manitol	16H29-B05-327813	2
Fagron	Manitol	16J28-B01-328593	2
Fagron	Manitol	16L15-B04	1
Fagron	Manitol	16L15-B04-329317	2
Fagron	Manitol	16L15-B05-329316	1
Fagron	Manitol	17/13-B04-340968	3
Fagron	Manitol	17/13-B10	1
Fagron	Manitol	17/13-B11-341331	1
Fagron	Manitol	17045002	1
Fagron	Manitol	170612185	1
Fagron	Manitol	17123B05342007	1
Fagron	Manitol	1713-B11	1
Fagron	Manitol	17A12-B02	1
Fagron	Manitol	17A12-B02-332068	2
Fagron	Manitol	17A12-B03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Manitol	17A12-B04-330729	1
Fagron	Manitol	17A12-Bo3	1
Fagron	Manitol	17A27-B02	1
Fagron	Manitol	17A27-B02-331292	4
Fagron	Manitol	17B08-B02	2
Fagron	Manitol	17B08-B04	3
Fagron	Manitol	17B08-B04_352402	1
Fagron	Manitol	17B08-B04-334312	2
Fagron	Manitol	17B08-B04-334313	1
Fagron	Manitol	17B08-B04-334314	1
Fagron	Manitol	17B08-B04-352402	5
Fagron	Manitol	17C28-B03-333349	1
Fagron	Manitol	17C28-B05333613	1
Fagron	Manitol	17C28-B06	2
Fagron	Manitol	17D12-B01-334435	6
Fagron	Manitol	17D18-B01	1
Fagron	Manitol	17D18-B03-335437	2
Fagron	Manitol	17E03-B01-336748	1
Fagron	Manitol	17F27-B03-337911	1
Fagron	Manitol	17F27B04337912	1
Fagron	Manitol	17F27B04-337912	1
Fagron	Manitol	17F27-B04-337912	2
Fagron	Manitol	17F27-B05-337913	1
Fagron	Manitol	17F27-B07	2
Fagron	Manitol	17F27-B07-338598	2
Fagron	Manitol	17F27-B08	1
Fagron	Manitol	17F27-B08-338599	1
Fagron	Manitol	17I13B03340967	1
Fagron	Manitol	17I13-B03-340967	2
Fagron	Manitol	17I13-B04-340968	1
Fagron	Manitol	17I13-B10	1
Fagron	Manitol	17I13-B11-341331	1
Fagron	Manitol	17J04-B06	1
Fagron	Manitol	17J04-B06-341798	2
Fagron	Manitol	17J04-B07-341800	1
Fagron	Manitol	17J23-B05	2
Fagron	Manitol	17J23-B05-342007	4
Fagron	Manitol	17J23-B06	1
Fagron	Manitol	17J30309-343413	1
Fagron	Manitol	17J30-B09-343413	2
Fagron	Manitol	17J30-B10-343414	2
Fagron	Manitol	17J30-B11-343939	1
Fagron	Manitol	17K29-B04-343940	1
Fagron	Manitol	17K29-B05	1
Fagron	Manitol	17K29-B05-345229	3
Fagron	Manitol	17K29-B07-344253	1
Fagron	Manitol	17L04-B03-345230	1
Fagron	Manitol	17L04-B04-345231	2
Fagron	Manitol	17L18-B04-351506	1
Fagron	Manitol	17LO4-B08	1
Fagron	Manitol	18/25-B08-356984	2
Fagron	Manitol	1806024-01	1
Fagron	Manitol	1830-08-346849	1
Fagron	Manitol	18A30-B06-346848	3
Fagron	Manitol	18A30-B07-348872	3
Fagron	Manitol	18A30-B08-346849	3
Fagron	Manitol	18A30-B09-346850	1
Fagron	Manitol	18A30-B10	1
Fagron	Manitol	18B23-B10-349553	3
Fagron	Manitol	18B23-B12-349972	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Manitol	18D09-B11	1
Fagron	Manitol	18D09-B11-351436	3
Fagron	Manitol	18D09-B13	1
Fagron	Manitol	18D09-B13-352214	2
Fagron	Manitol	18D09-B15-352216	1
Fagron	Manitol	18D09-B16-352503	1
Fagron	Manitol	18E25-B05-352504	2
Fagron	Manitol	18E25-B06-352505	2
Fagron	Manitol	18E25-B07	1
Fagron	Manitol	18E25-B07-352753	1
Fagron	Manitol	18E25-B-07-352753	1
Fagron	Manitol	18E25-B08	1
Fagron	Manitol	18E25-B08-352754	1
Fagron	Manitol	18E25B09352755	1
Fagron	Manitol	18E25-B09-352755	4
Fagron	Manitol	18g04-813-3541621	1
Fagron	Manitol	18G04-B09	1
Fagron	Manitol	18G04-B10-354321	2
Fagron	Manitol	18G04-B11-354322	1
Fagron	Manitol	18G04-B13	2
Fagron	Manitol	18G04-B13-354621	6
Fagron	Manitol	18H16-B01-357217	2
Fagron	Manitol	18H16-B01-359311	1
Fagron	Manitol	18H16-B01-3633309	1
Fagron	Manitol	18H16-B01-365268	1
Fagron	Manitol	18J04-B05-355467	4
Fagron	Manitol	18j04B07-355587	1
Fagron	Manitol	18J04-B07-355587	1
Fagron	Manitol	18J04-B10-355589	1
Fagron	Manitol	18J25-B05-356984	1
Fagron	Manitol	18J25-B07-356983	1
Fagron	Manitol	18J25-B08	1
Fagron	Manitol	18J25-B08-356984	3
Fagron	Manitol	18L03-B03	3
Fagron	Manitol	18L03-B03-357463	2
Fagron	Manitol	18L03-B06-357782	1
Fagron	Manitol	18L21-B03	1
Fagron	Manitol	18L21-B03-358869	1
Fagron	Manitol	18L21-B04-358870	2
Fagron	Manitol	18L21-B04-358879	1
Fagron	Manitol	18L21-B05	1
Fagron	Manitol	18L21-B05-358871	5
Fagron	Manitol	18L21-B06-3558872	1
Fagron	Manitol	18L21-B06-358872	1
Fagron	Manitol	18L21-B08-358874	1
Fagron	Manitol	19/19-F10-366892	1
Fagron	Manitol	19/20-F07-366390	1
Fagron	Manitol	19/20-F12-366393	1
Fagron	Manitol	19120-F09-366392	1
Fagron	Manitol	19120F13366394	1
Fagron	Manitol	19120-F15-366395	1
Fagron	Manitol	19A14-B03-360504	2
Fagron	Manitol	19A14-B04_360505	1
Fagron	Manitol	19A14B04360505	1
Fagron	Manitol	19A14-B04-360505	4
Fagron	Manitol	19A14-B05-360506	1
Fagron	Manitol	19A14-B06-360507	1
Fagron	Manitol	19B12-B02	2
Fagron	Manitol	19B12-B02-359604	1
Fagron	Manitol	19B12-B03-059605	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Manitol	19B12-B03-359605	1
Fagron	Manitol	19C11B02361201	1
Fagron	Manitol	19C11B02-361201	1
Fagron	Manitol	19C11-B02-361201	2
Fagron	Manitol	19C11-B03-361202	1
Fagron	Manitol	19C11B04361203	1
Fagron	Manitol	19C11-B04-361203	1
Fagron	Manitol	19C11-B05-361204	1
Fagron	Manitol	19C14-B02-361206	1
Fagron	Manitol	19C14-B06321213	1
Fagron	Manitol	19c14-B06-361213	1
Fagron	Manitol	19D16-B03	1
Fagron	Manitol	19D16-B03-364401	3
Fagron	Manitol	19D16-B04-364402	1
Fagron	Manitol	19D16-B05	1
Fagron	Manitol	19E06-B05-363487	3
Fagron	Manitol	19E06B06363488	1
Fagron	Manitol	19E06-B06-363488	6
Fagron	Manitol	19E06-B08-363490	1
Fagron	Manitol	19F12-B09-363871	3
Fagron	Manitol	19F12-B10-363872	3
Fagron	Manitol	19F12-B11	1
Fagron	Manitol	19F12-b11-363873	1
Fagron	Manitol	19F12-B11-363873	1
Fagron	Manitol	19I19-F1	1
Fagron	Manitol	19I19-F10	1
Fagron	Manitol	19I19-F10-366892	3
Fagron	Manitol	19I19-F11-366893	1
Fagron	Manitol	19I19-F14-366950	2
Fagron	Manitol	19I20_F13-366394	1
Fagron	Manitol	19I20-F09	1
Fagron	Manitol	19I20-F09-366392	1
Fagron	Manitol	19I20-F12-366393	2
Fagron	Manitol	19I20-F13	1
Fagron	Manitol	19i20-f15	1
Fagron	Manitol	19I20-F15	1
Fagron	Manitol	19I20-F15-366395	4
Fagron	Manitol	19J09-F03	1
Fagron	Manitol	19J09-F08-366955	2
Fagron	Manitol	20006F20375113	1
Fagron	Manitol	20B05-04-369845	1
Fagron	Manitol	20B05-F03	3
Fagron	Manitol	20B05-F04	1
Fagron	Manitol	20B05F04369845	2
Fagron	Manitol	20B05-F05-369846	1
Fagron	Manitol	20B05-F06	1
Fagron	Manitol	20B05-F06-369847	1
Fagron	Manitol	20C06-F06	1
Fagron	Manitol	20C06-F06-369853	1
Fagron	Manitol	20C06-F07-369854	1
Fagron	Manitol	20D16F11	1
Fagron	Manitol	20D16-F11-371552	2
Fagron	Manitol	20D16-F12	2
Fagron	Manitol	20D16-F12-371553	4
Fagron	Manitol	20D16-F13-371555	5
Fagron	Manitol	20D16F14371554	1
Fagron	Manitol	20D16-F15	1
Fagron	Manitol	20E25-F06-372224	1
Fagron	Manitol	20E25-F07-372221	5
Fagron	Manitol	20E25-F08-372222	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Manitol	20F12_F06_373767	1
Fagron	Manitol	20F12-F06-373767	3
Fagron	Manitol	20F12-F07	1
Fagron	Manitol	20F12-F07-373768	2
Fagron	Manitol	20F12-F08	2
Fagron	Manitol	20F12-F08-373769	1
Fagron	Manitol	20F12-F09-373770	3
Fagron	Manitol	20F12-F10-373771	2
Fagron	Manitol	20F12-F15-373776	1
Fagron	Manitol	20F12-F-373768	1
Fagron	Manitol	20H21-06	1
Fagron	Manitol	20H21-F03	1
Fagron	Manitol	20H21-F03-373847	3
Fagron	Manitol	20H21-F04-373848	5
Fagron	Manitol	20H21-F05-373849	1
Fagron	Manitol	20H21-F06-373987	5
Fagron	Manitol	20H21-F08-373989	2
Fagron	Manitol	20H21-F09	1
Fagron	Manitol	20H21-F09-373990	1
Fagron	Manitol	20J06F13	1
Fagron	Manitol	20J06-F13	1
Fagron	Manitol	20J06-F14-375107	2
Fagron	Manitol	20J06-F15-375108	3
Fagron	Manitol	20J06-F16	2
Fagron	Manitol	20J06-F21-375114	2
Fagron	Manitol	20L1115-F10-376720	1
Fagron	Manitol	20L15-F10	1
Fagron	Manitol	20L15-F10-376720	2
Fagron	Manitol	20L15-F15-376869	2
Fagron	Manitol	21B12F04377243	1
Fagron	Manitol	21B12-F04-377243	3
Fagron	Manitol	21C31-F04-378222	4
Fagron	Manitol	21C31-F06	1
Fagron	Manitol	21C31F04	1
Fagron	Manitol	21D02F05	1
Fagron	Manitol	21D02-F05	1
Fagron	Manitol	21D02-F06-378226	4
Fagron	Manitol	21E25-F07	1
Fagron	Manitol	21E25f07-379700	1
Fagron	Manitol	21E25-F07-379700	2
Fagron	Manitol	21E25-F08-379701	3
Fagron	Manitol	21f16f05379703	1
Fagron	Manitol	21H04-F05	3
Fagron	Manitol	21H04-F05-379996	1
Fagron	Manitol	21K10-F01-380693	1
Fagron	Manitol	21K10-F04	2
Fagron	Manitol	21K16-B11-216336	2
Fagron	Manitol	22822F-06	1
Fagron	Manitol	22A12-F05-381468	2
Fagron	Manitol	22A12-F07-381470	2
Fagron	Manitol	22A12-F09-381478	1
Fagron	Manitol	22A12-F14	1
Fagron	Manitol	22A12-F14-381239	3
Fagron	Manitol	22B01-F04	1
Fagron	Manitol	22B01-F04-381542	2
Fagron	Manitol	22B22-F06-381606	5
Fagron	Manitol	22B22F08	1
Fagron	Manitol	22B22-F08-381608	2
Fagron	Manitol	22B22-F13	1
Fagron	Manitol	22B22-F13-381720	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Manitol	22B22-F14-381721	1
Fagron	Manitol	22B22-F15	1
Fagron	Manitol	22B22-F15-381722	4
Fagron	Manitol	22e23f12	1
Fagron	Manitol	22E23-F12-382118	1
Fagron	Manitol	22E23-F13-382119	3
Fagron	Manitol	22E23-F14	3
Fagron	Manitol	22E23-F14-382120	3
Fagron	Manitol	22E23-F15	2
Fagron	Manitol	22E23-F15-382121	1
Fagron	Manitol	22E23-F17-382114	1
Fagron	Manitol	22E23F18382115	1
Fagron	Manitol	22E23-F19-382117	5
Fagron	Manitol	22E23-F21-382116	2
Fagron	Manitol	22E23F-F06	1
Fagron	Manitol	22F15-F10-382723	1
Fagron	Manitol	22F15-F12-382724	1
Fagron	Manitol	22F15F15382727	1
Fagron	Manitol	22F15-F15-382727	1
Fagron	Manitol	22F15F16382728	1
Fagron	Manitol	22F15-F17-382731	1
Fagron	Manitol	22F15-F18-382732	1
Fagron	Manitol	22F15-F20	1
Fagron	Manitol	22F15-F20-382742	2
Fagron	Manitol	23A10_F03_384081	1
Fagron	Manitol	23A10-F07-384082	1
Fagron	Manitol	23A10-F09-384083	2
Fagron	Manitol	23A10-F09-384303	1
Fagron	Manitol	23A10-F14-384085	1
Fagron	Manitol	23a24-f03-384303	1
Fagron	Manitol	23A24-F13-384485	1
Fagron	Manitol	296196	1
Fagron	Manitol	4092019Mi	1
Fagron	Manitol	5-37970003	1
Fagron	Manitol	6E11-B08-323540	1
Fagron	Manitol	720014-0001	2
Fagron	Manitol	720014-0002	1
Fagron	Manitol	B04-3524002	1
Fagron	Manitol	E166K/21K16-B11-216336	1
Fagron	Manitol	E611X	1
Fagron	Manitol	E833Z	1
Fagron	Manitol	E911K	1
Fagron	Manitol	f07-3814700	1
Fagron	Manitol	F08-3737609	1
Fagron	Manitol	F09-3737700	1
Fagrron	Manitol	17C28-B05-33361	1
Fargon - Alliance He…	Manitol	19I20-F13-366394	1
Fargon / Noweda	Manitol	20J06-F20	1
Fargon/ Noweda	Manitol	15A26-B01-304717	1
Fargon/ Phoenix	Manitol	19I20-F13-366394	1
Fargon/Noweda	Manitol	19016-B03	1
Fargon	Manitol	12E24-N08	1
Fargon	Manitol	18B23-B10-349553	1
Fargon	Manitol	18D09-B16-352503	1
Fiebig/Farago	Manitol	19E06-B06-363488	1
FIEBIG	Manitol	191654012	1
Fischar/Noweda	Manitol	18E25-B09	1
Fragon/ Gehe	Manitol	18103b06357782	1
Fragon	Manitol	18D09-B13-352214	1
FragonFiebig	Manitol	18A30-B07-348872	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fragron/ Alliance	Manitol	19C11-B04	1
Fragron/Noweda	Manitol	17A12-B04-330729	1
Gatt-Koller	Manitol	1803827	2
gehe 10.12.13	Manitol	1305043/01	1
GEHE 24.07.2014	Manitol	1310004-02	1
Gehe/ Eurho	Manitol	1205016-02	1
Gehe/Euro	Manitol	1511025-01	1
Gehe	Manitol	12E24-N08	1
Gehe	Manitol	12J26-N15	1
GEHE	Manitol	130504301	1
Gehe	Manitol	13E24-N01	1
Gehe	Manitol	150202201	1
Gehe	Manitol	1508012-01	1
Gehe	Manitol	15197313	1
Gehe	Manitol	1606031-01	1
Gehe	Manitol	16200913	1
Gehe	Manitol	17045009	1
GEHE	Manitol	17258808	1
Gehe	Manitol	17258812	1
Gehe	Manitol	17360101	2
GEHE	Manitol	17B08-B04-334312	1
Gehe	Manitol	17F27-B05-337913	1
Gehe	Manitol	17L04-B03-345230	1
Gehe	Manitol	1908019-01	1
Gehe	Manitol	19B12-B02-359604	1
Gehe	Manitol	2008030-01	1
Gehe	Manitol	21003432002	1
Gehe	Manitol	2108014-01	2
Gehe	Manitol	21K16-B11-216336	1
Gehe	Manitol	22001495041	1
Gehe	Manitol	22001712012	1
Gehe	Manitol	2209020-01	1
Gehe	Manitol	23A10-F13-384085	1
Gutenberg-Apotheke	Manitol	1310004-01	4
Gutenberg-Apotheke	Manitol	1310004-02	1
Gutenberg-Apotheke	Manitol	13189221	1
Hirsch	Manitol	12305725	1
INTERN-DROGEN	Manitol	17258812	1
JENNE	Manitol	17258811	1
Jenne	Manitol	24000356001	3
Kehr 15.09.2020	Manitol	20B05-F03-369844	1
Kehr	Manitol	22F15-F18	1
Kehr	Manitol	2307004-01	2
Klenk	Manitol	1211034-02	2
Klenk	Manitol	1606031-01	2
Klenk	Manitol	17360108	1
Klenk	Manitol	5224A110314	1
Kögl	Manitol	1900820	1
Krieger	Manitol	20F12-F10-373771	1
Krieger	Manitol	20L15-F15-376869	1
Linden-Apotheke	Manitol	1205016-02	1
Noewda	Manitol	15197319	1
Noweda Frechen	Manitol	20J06F13375106	1
Noweda/Fragron	Manitol	18E25-B07-352753	1
Noweda/Fragron	Manitol	19D16-B04	1
Noweda	Manitol	11219101	2
Noweda	Manitol	11219138	1
Noweda	Manitol	1205016-02	2
Noweda	Manitol	12105404	1
Noweda	Manitol	1305043-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Manitol	14323124	1
Noweda	Manitol	1508012-01	1
Noweda	Manitol	1511025-01	1
Noweda	Manitol	15B05-B06-304302	1
Noweda	Manitol	15I24-B05-314323	1
Noweda	Manitol	15K17-B01	1
Noweda	Manitol	15l24-B05-314323	1
Noweda	Manitol	16D20-B04-320487	1
Noweda	Manitol	16L15-B05-329316	1
Noweda	Manitol	17045002	1
Noweda	Manitol	1708005-01	3
Noweda	Manitol	17258812	1
Noweda	Manitol	1809008-02	1
Noweda	Manitol	18B23-B10	1
Noweda	Manitol	18L03-B06-357782	1
Noweda	Manitol	1904025-01	1
Noweda	Manitol	19D16-B03	1
Noweda	Manitol	20004038003	1
Noweda	Manitol	21K16-B11-216336	1
Noweda	Manitol	22001712011	1
Noweda	Manitol	2201036-01	1
Noweda	Manitol	23A10-F03	1
Noweda	Manitol	P101P102P103	3
Noweda29.04.2015	Manitol	14323113	1
Phagron	Manitol	1302C004-279405	1
PHOENIX 24.04.2014	Manitol	1310004-01	3
Phoenix WE 10.03.17 ...	Manitol	16340302	1
Phoenix/Fragon	Manitol	17B08-B04-334314	1
Phoenix	Manitol	120501602	1
Phoenix	Manitol	1310004-01	1
Phoenix	Manitol	15197314	1
Phoenix	Manitol	15197319	1
Phoenix	Manitol	1708005-01	2
Phoenix	Manitol	18265503	1
Phoenix	Manitol	18265506	1
Phoenix	Manitol	18L21-B04-358870	1
Phoenix	Manitol	19B12-B03	1
Phoenix	Manitol	19C11-B03-361202	1
Phoenix	Manitol	20000958001	1
Phoenix	Manitol	20003605013	1
Phoenix	Manitol	200180502	1
Phoenix	Manitol	200331404	1
Phönix WE:02.08.201...	Manitol	15197313	1
Phönix Gotha	Manitol	19I20-F09	1
Phönix/ Caesar&Loret...	Manitol	20000958003	1
Phönix	Manitol	120501602	1
Phönix	Manitol	1211034-02	1
Phönix	Manitol	12305723	1
Phönix	Manitol	1305043-01	1
Phönix	Manitol	14051215	1
phönix	Manitol	14323138	1
phönix	Manitol	15197313	2
PHÖNIX	Manitol	16200923	1
Phönix	Manitol	16200924	2
PHÖNIX	Manitol	16212102	1
Phönix	Manitol	17045008	1
Phönix	Manitol	17258819	1
PHÖNIX	Manitol	17258821	1
PHÖNIX	Manitol	17258823	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Manitol	17360109	1
Phönix	Manitol	18265411	1
Phönix	Manitol	18265429	1
Phönix	Manitol	18L21-B04	1
Phönix	Manitol	20H21-F06-373986	1
Phönix	Manitol	22822-F08	1
PHÖNIX	Manitol	22A12F04-381467	1
Phönix	Manitol	23A10-F14-384085	1
Primavera/Phoenix	Manitol	1708005-01	1
Retest	Manitol	1409016-01	1
Roquette / Gehe	Manitol	E851E	1
Roquette Lestrem/Noweda	Manitol	1508012-01	1
Roquette Lestrem/Noweda	Manitol	1511025-01	1
Roquette/Noweda	Manitol	E235L	1
Roquette/Phoenix	Manitol	E118T	1
Sana	Manitol	17258809	2
Sanac	Manitol	1610027-01	1
Sanacorp E.K:19,49 ...	Manitol	17045009	1
Sanacorp 06.05.22 18,91EUR	Manitol	22B01-F04-381542	1
Sanacorp	Manitol	10974140	1
Sanacorp	Manitol	1310004-01	1
Sanacorp	Manitol	13189215	1
Sanacorp	Manitol	14051205	1
Sanacorp	Manitol	16200903	1
Sanacorp	Manitol	16200924	1
Sanacorp	Manitol	17087916	1
Sanacorp	Manitol	17258808	1
Sanacorp	Manitol	17258809	1
Sanacorp	Manitol	17K29-B05	1
Sanacorp	Manitol	1806024-01	1
Sanacorp	Manitol	18265509	1
Sanacorp	Manitol	1904025-02	1
Sanacorp	Manitol	22001712004	1
Sanacorp	Manitol	22001712011	2
Sanacorp	Manitol	2201712011	1
Sanacorp	Manitol	22E23-F18-382115	1
Sanacorp	Manitol	2301038-01	1
Sanacorp	Manitol	23A24-F03-384303	1
Sanacorp	Manitol	24000356003	1
Sanacorp	Manitol	24000356005	1
Sancorp/Euro OCT	Manitol	190425-02	1
Shijiazhuang/Phoenix	Manitol	1901092	2
Sonnen-Apotheke Wefe...	Manitol		2
Sonnen-Apotheke Wefe...	Manitol	4/2021	1
stumpf	Manitol	1104028-02	1
VDL;21.11.14;3,98EUR	Manitol	13189227	1
vwr chemicals	Manitol	20K134121	1
vwr chemicals	Manitol	21G264113	1
WE:16.03.2016 Sanacorp	Manitol	14323124	1
WE:30.03.2016 Sanacorp	Manitol	14323138	1
WE:Sanacorp 02.09.16...	Manitol	16212101	1
WE:Sanacorp 25.10.20...	Manitol	16212102	2
xxxxx	Manitol	xxxx	1

- 232 796 spectra from 1515 *Apo-Ident* customers from a total of 48 394 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Manitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Manitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	1670	0	200 334
Type C	0	3267	4	232 773

The substance/substance group *Manitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6407 %)
Type C	100.0000 % (> 99.9005 %)	99.8777 % (> 99.7860 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20980	20980	0,00	176,70
21884	21884	0,00	177,19
22286	22286	0,00	177,46
22581	22286	2,81	180,01
22883	22286	4,40	178,69
22884	22286	4,98	178,25
24579	21884	7,81	187,39
25548	25548	0,00	178,84
26396	22286	12,81	193,04

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Melatonina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20553-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Melatonina; Melatoninum

Special notes

When selecting the *Melatonina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Melatonina	11	13	332

Second-stage model

For differentiation of the substance/substance group *Melatonina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Melatonina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	84,77	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Melatonina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Melatonina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Melatonina	12321404	20834	40	20121107
Caelo	Melatonina	12321411	20835	40	20121107
Caelo	Melatonina	12321415	20987	80	20121107
Caelo	Melatonina	21002239029	26415	40	20210723
Caelo	Melatonina	21002239029	26415SI	40	20210723
Euro OTC	Melatonina	1305029-02	21618	60	1411054
Euro OTC	Melatonina	1510041	22237	60	20151123*
Euro OTC	Melatonina	1709020	23889	40	20180105*
Euro OTC	Melatonina	1804015	24128	40	20180522*
Euro OTC	Melatonina	1804015	24128SI	40	20180522*
Euro OTC	Melatonina	2101018	25542	40	20210202*
Euro OTC	Melatonina	2101018	25542SI	40	20210202*
Fagron	Melatonina	15G06-B03-315183	22892	40	20150717
Fagron	Melatonina	15G06-B03-323733	22893	40	20150717

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 640 spectra of 14 reference samples from the substance/substance group *Melatonina*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 322 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1019 spectra of 25 reference samples from the substance/substance group *Melatonina*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Melatonina	163437	23036	40
Caelo	Melatonina	190946	24519	40
Caelo	Melatonina	22003650	26487	40
Euro OTC	Melatonina	1610040	22871	40
Euro OTC	Melatonina	1811004	24330	40
Euro OTC	Melatonina	1906031	24767	40
Euro OTC	Melatonina	1906030	24802	40
Euro OTC	Melatonina	1909031	24924	40
Euro OTC	Melatonina	2002029	25148	40
Euro OTC	Melatonina	2106005	25766	50
Euro OTC	Melatonina	2110002	25890	50
Euro OTC	Melatonina	2309003	27283	40
Fagron	Melatonina	22I16-B05-224268	26458	40
Caelo	Melatonina	163437	23036SI	40
Caelo	Melatonina	190946	24519SI	40
Caelo	Melatonina	22003650	26487SI	40
Euro OTC	Melatonina	1510041	22237SI†	60
Euro OTC	Melatonina	1811004	24330SI	39
Euro OTC	Melatonina	2002029	25148SI	40
Euro OTC	Melatonina	2106005	25766SI	50
Euro OTC	Melatonina	2110002	25890SI	10
Euro OTC	Melatonina	2309003	27283SI	40
Fagron	Melatonina	15G06-B03-315183	22892SI†	40
Fagron	Melatonina	15G06-B03-323733	22893SI†	40
Fagron	Melatonina	22I16-B05-224268	26458SI	40

- 201 065 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1695 spectra from 478 *Apo-Ident* customers from 342 batches from the substance/substance group *Melatonina*.

- Among them are spectra of independent samples from 332 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Melatonina	192978006	2
	Melatonina	20220508	1
	Melatonina	20A31-F02-372824	1
	Melatonina	20A31-F02-377484	2
	Melatonina	21002239013	1
	Melatonina	21002239023	1
	Melatonina	21002239028	2
	Melatonina	21002239030	4
	Melatonina	21002239034	1
	Melatonina	21002239035	1
	Melatonina	21002239038	11
	Melatonina	21002239039	3
	Melatonina	21002239041	1
	Melatonina	2110002-01	5
	Melatonina	22003650002	11
	Melatonina	22003650004	2
	Melatonina	22003650005	3
	Melatonina	22003650009	1
	Melatonina	22003650011	2
	Melatonina	22003650014	1
	Melatonina	2203650003	1
	Melatonina	22116-B05-228535	1
	Melatonina	22I16-B05-228535	1
	Melatonina	22I16-B05-228536	1
	Melatonina	22I16-B05-235144	1
	Melatonina	2309003-01	1
	Melatonina	B05-2285306	1
AEP	Melatonina	20001543005	1
AHD	Melatonina	21002239018	1
AHD	Melatonina	21002239038	3
AHD	Melatonina	22003650005	1
Alcon Biosciences Pr...	Melatonina	APALC/MLT/170301M	1
Alliance	Melatonina	15254307	3
Alliance	Melatonina	15254316	1
Alliance	Melatonina	21002239025	1
allianz	Melatonina	15254324	1
Alte Apotheke	Melatonina	15254328	1
Anzag	Melatonina	12321415	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
apo ident	Melatonina	1610040-02	1
Audor Pharma	Melatonina	ALC/MLT/170901	1
Audor Pharma	Melatonina	APALC/MLT/150501M	2
Audor Pharma	Melatonina	APALC/MLT/170901M	2
Audor Pharma	Melatonina	APALC/MLT/17090M	1
Bionorica Ethics	Melatonina	APALC/MLT/170901M	1
Bombastus	Melatonina	18210304	1
Caelo	Melatonina		1
Caelo	Melatonina	1(20001543007)	1
Caelo	Melatonina	10071303	1
Caelo	Melatonina	1126109	1
Caelo	Melatonina	11267102	1
Caelo	Melatonina	11267109	1
Caelo	Melatonina	11267110	1
Caelo	Melatonina	11267111	1
Caelo	Melatonina	11267119	1
Caelo	Melatonina	11267120	4
Caelo	Melatonina	11267121	1
Caelo	Melatonina	11267122	1
Caelo	Melatonina	11267126	2
Caelo	Melatonina	117305118	1
Caelo	Melatonina	120009	1
Caelo	Melatonina	12321404	3
Caelo	Melatonina	12321406	1
Caelo	Melatonina	12321411	1
Caelo	Melatonina	12321415	3
Caelo	Melatonina	12321416	5
Caelo	Melatonina	12321421	2
Caelo	Melatonina	12321422	4
Caelo	Melatonina	13167301	8
Caelo	Melatonina	13167302	1
Caelo	Melatonina	13167309	1
Caelo	Melatonina	13167310	1
Caelo	Melatonina	13167312	3
Caelo	Melatonina	13167314	5
Caelo	Melatonina	14110302	2
Caelo	Melatonina	14110305	2
Caelo	Melatonina	14110308	3
Caelo	Melatonina	14110314	2
Caelo	Melatonina	14110316	1
Caelo	Melatonina	150601	1
Caelo	Melatonina	15093001	7
Caelo	Melatonina	15093002	2
Caelo	Melatonina	15093004	2
Caelo	Melatonina	15093008	8
Caelo	Melatonina	15093010	5
Caelo	Melatonina	15093012	2
Caelo	Melatonina	15093013	2
Caelo	Melatonina	1514E-03554	1
Caelo	Melatonina	1524309	1
Caelo	Melatonina	15254305	7
Caelo	Melatonina	15254306	8
Caelo	Melatonina	15254307	14
Caelo	Melatonina	15254308	7
Caelo	Melatonina	15254313	2
Caelo	Melatonina	15254319	10
Caelo	Melatonina	15254320	4
Caelo	Melatonina	15254321	8
Caelo	Melatonina	15254324	4
Caelo	Melatonina	15254325	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melatonina	15254327	1
Caelo	Melatonina	15254328	2
Caelo	Melatonina	15254331	8
Caelo	Melatonina	15254332	2
Caelo	Melatonina	15254333	1
Caelo	Melatonina	15254336	4
Caelo	Melatonina	15254338	6
Caelo	Melatonina	15C20B01306077	1
Caelo	Melatonina	15G06-B03-321298	2
Caelo	Melatonina	15G06-B03-321299	1
Caelo	Melatonina	15G06-B03-323733	1
Caelo	Melatonina	160125M	1
Caelo	Melatonina	16121303	1
Caelo	Melatonina	16266901	9
Caelo	Melatonina	16266903	2
Caelo	Melatonina	16266904	3
Caelo	Melatonina	16266906	4
Caelo	Melatonina	16266908	7
Caelo	Melatonina	16266909	10
Caelo	Melatonina	16266912	2
Caelo	Melatonina	163437/13	1
Caelo	Melatonina	16343702	3
Caelo	Melatonina	16343705	2
Caelo	Melatonina	16343706	2
Caelo	Melatonina	16343707	2
Caelo	Melatonina	16343708	13
Caelo	Melatonina	16343709	13
Caelo	Melatonina	16343710	12
Caelo	Melatonina	16343711	4
Caelo	Melatonina	16343712	1
Caelo	Melatonina	16343713	12
Caelo	Melatonina	17/28-B04-345376	2
Caelo	Melatonina	17/28-b04-351312	1
Caelo	Melatonina	1709020-01	2
Caelo	Melatonina	17305101	5
Caelo	Melatonina	17305101-20180206Ma1	1
Caelo	Melatonina	17305102	30
Caelo	Melatonina	17305104	4
Caelo	Melatonina	17305105	15
Caelo	Melatonina	17305106	13
Caelo	Melatonina	17305109	1
Caelo	Melatonina	17305110	7
Caelo	Melatonina	17305113	7
Caelo	Melatonina	17305114	8
Caelo	Melatonina	17305115	5
Caelo	Melatonina	17305116	4
Caelo	Melatonina	17305118	13
Caelo	Melatonina	17305119	6
Caelo	Melatonina	17305120	1
Caelo	Melatonina	17305121	5
Caelo	Melatonina	17305122	14
Caelo	Melatonina	17350119	1
Caelo	Melatonina	17C22-B01-337090	1
Caelo	Melatonina	17I28-B04-344439	2
Caelo	Melatonina	17I28-B04-345376	1
Caelo	Melatonina	17l28-B04-351312	1
Caelo	Melatonina	1810308	1
Caelo	Melatonina	182010312	1
Caelo	Melatonina	18210301	18
Caelo	Melatonina	18210303	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melatonina	18210304	19
Caelo	Melatonina	18210306	11
Caelo	Melatonina	18210307	4
Caelo	Melatonina	18210308	5
Caelo	Melatonina	18210311	14
Caelo	Melatonina	18210312	10
Caelo	Melatonina	18210313	8
Caelo	Melatonina	18210315	1
Caelo	Melatonina	18210318	11
Caelo	Melatonina	18210319	4
Caelo	Melatonina	191280001	17
Caelo	Melatonina	191280002	12
Caelo	Melatonina	191280003	1
Caelo	Melatonina	191280005	17
Caelo	Melatonina	191280006	2
Caelo	Melatonina	191280009	16
Caelo	Melatonina	19128001	1
Caelo	Melatonina	19128003	10
Caelo	Melatonina	19128005	18
Caelo	Melatonina	19128006	20
Caelo	Melatonina	19128007	11
Caelo	Melatonina	192978004	1
Caelo	Melatonina	192978005	16
Caelo	Melatonina	192978006	17
Caelo	Melatonina	2(20001543007)	1
Caelo	Melatonina	20001543005	8
Caelo	Melatonina	20001543007	12
Caelo	Melatonina	20001543009	1
Caelo	Melatonina	20001543010	10
Caelo	Melatonina	20001543012	11
Caelo	Melatonina	20001543014	16
Caelo	Melatonina	20021312	1
Caelo	Melatonina	20021505	1
Caelo	Melatonina	2002239003	1
Caelo	Melatonina	20A31-F02-372823	1
Caelo	Melatonina	21000597001	10
Caelo	Melatonina	21000597002	1
Caelo	Melatonina	21000597003	1
Caelo	Melatonina	21002239001	1
Caelo	Melatonina	21002239003	20
Caelo	Melatonina	21002239004	2
Caelo	Melatonina	21002239005	15
Caelo	Melatonina	21002239006	8
Caelo	Melatonina	21002239008	1
Caelo	Melatonina	21002239011	8
Caelo	Melatonina	21002239013	19
Caelo	Melatonina	21002239018	3
Caelo	Melatonina	21002239021	17
Caelo	Melatonina	21002239023	10
Caelo	Melatonina	21002239028	5
Caelo	Melatonina	21002239029	7
Caelo	Melatonina	21002239030	2
Caelo	Melatonina	21002239034	9
Caelo	Melatonina	21002239035	5
Caelo	Melatonina	21002239036	3
Caelo	Melatonina	21002239039	1
Caelo	Melatonina	2100223909	1
Caelo	Melatonina	2100597002	1
Caelo	Melatonina	211002239028	1
Caelo	Melatonina	22003650002	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melatonina	22003650005	1
Caelo	Melatonina	2313M03554	1
Caelo	Melatonina	2548268	1
Caelo	Melatonina	26051805	1
Caelo	Melatonina	ALC/MLT/170901	1
Caesa / Alliance Hea…	Melatonina	18210306	1
Caesar & Lorenz GmbH	Melatonina	17305106	1
Caesar & Loretz GmbH…	Melatonina	21002239013	1
Caesar & Loretz GmbH…	Melatonina	21002239035	1
Caesar & Loretz GmbH…	Melatonina	17305102	2
Caesar & Loretz GmbH…	Melatonina	17305106	1
Caesar & Loretz GmbH…	Melatonina	18210306	1
Caesar & Loretz GmbH…	Melatonina	21002239029	1
Caesar & Loretz GmbH…	Melatonina	20001543012	2
Caesar & Loretz GmbH…	Melatonina	20001543014	1
Caesar & Loretz GmbH/AHD	Melatonina	20001543010	1
Caesar & Loretz GmbH/AHD	Melatonina	21002239013	1
Caesar & Loretz GmbH…	Melatonina	192978006	4
Caesar & Loretz GmbH…	Melatonina	20001543007	2
Caesar & Loretz GmbH…	Melatonina	20001543009	1
Caesar & Loretz GmbH/Gehe	Melatonina	192978006	3
Caesar & Loretz GmbH/Gehe	Melatonina	20001543007	2
Caesar & Loretz GmbH/Gehe	Melatonina	20001543009	1
Caesar & Loretz GmbH/Gehe	Melatonina	20001543012	1
Caesar & Loretz GmbH/Gehe	Melatonina	21002239003	1
Caesar & Loretz GmbH/Gehe	Melatonina	21002239020	1
Caesar & Loretz GmbH/Gehe	Melatonina	21002239039	2
Caesar & Loretz GmbH/Gehe	Melatonina	22003650002	1
Caesar & Loretz GmbH…	Melatonina	192978004	1
Caesar & Loretz GmbH…	Melatonina	21000597002	1
Caesar & Loretz GmbH…	Melatonina	21002239021	2
Caesar & Loretz GmbH…	Melatonina	21002239030	1
Caesar & Loretz GmbH…	Melatonina	192978006	1
Caesar & Loretz GmbH…	Melatonina	21002239005	2
Caesar & Loretz GmbH…	Melatonina	191280005	1
Caesar & Loretz GmbH…	Melatonina	21002239011	1
Caesar & Loretz GmbH…	Melatonina	20001543010	1
Caesar & Loretz GmbH…	Melatonina	21002239008	1
Caesar & Loretz GmbH…	Melatonina	21002239013	1
Caesar & Loretz GmbH	Melatonina	1524517305113	1
Caesar & Loretz GmbH	Melatonina	17305105	1
Caesar & Loretz GmbH	Melatonina	17305106	1
Caesar & Loretz GmbH	Melatonina	17305118	1
Caesar & Loretz GmbH	Melatonina	18210301	2
Caesar & Loretz GmbH	Melatonina	18210304	1
Caesar & Loretz GmbH	Melatonina	18210305	2
Caesar & Loretz GmbH	Melatonina	18210306	1
Caesar & Loretz GmbH	Melatonina	18210307	1
Caesar & Loretz GmbH	Melatonina	18210311	2
Caesar & Loretz GmbH	Melatonina	18210312	2
Caesar & Loretz GmbH	Melatonina	18210313	1
Caesar & Loretz GmbH	Melatonina	18210318	2
Caesar & Loretz GmbH	Melatonina	18210319	1
Caesar & Loretz GmbH	Melatonina	18210320	1
Caesar & Loretz GmbH	Melatonina	191280001	6
Caesar & Loretz GmbH	Melatonina	191280002	4
Caesar & Loretz GmbH	Melatonina	191280003	1
Caesar & Loretz GmbH	Melatonina	191280005	7
Caesar & Loretz GmbH	Melatonina	191280006	3
Caesar & Loretz GmbH	Melatonina	191280008	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Melatonina	191280009	7
Caesar & Loretz GmbH	Melatonina	19128003	1
Caesar & Loretz GmbH	Melatonina	19128005	5
Caesar & Loretz GmbH	Melatonina	19128007	2
Caesar & Loretz GmbH	Melatonina	192978004	4
Caesar & Loretz GmbH	Melatonina	192978005	5
Caesar & Loretz GmbH	Melatonina	192978006	16
Caesar & Loretz GmbH	Melatonina	20001543005	3
Caesar & Loretz GmbH	Melatonina	20001543007	1
Caesar & Loretz GmbH	Melatonina	20001543009	1
Caesar & Loretz GmbH	Melatonina	20001543010	3
Caesar & Loretz GmbH	Melatonina	20001543012	5
Caesar & Loretz GmbH	Melatonina	20001543014	11
Caesar & Loretz GmbH	Melatonina	2002029-01	2
Caesar & Loretz GmbH	Melatonina	21000597001	5
Caesar & Loretz GmbH	Melatonina	21000597002	2
Caesar & Loretz GmbH	Melatonina	21002239003	3
Caesar & Loretz GmbH	Melatonina	21002239004	3
Caesar & Loretz GmbH	Melatonina	21002239005	11
Caesar & Loretz GmbH	Melatonina	21002239006	4
Caesar & Loretz GmbH	Melatonina	21002239008	1
Caesar & Loretz GmbH	Melatonina	21002239013	9
Caesar & Loretz GmbH	Melatonina	21002239018	2
Caesar & Loretz GmbH	Melatonina	21002239020	2
Caesar & Loretz GmbH	Melatonina	21002239021	7
Caesar & Loretz GmbH	Melatonina	21002239023	6
Caesar & Loretz GmbH	Melatonina	21002239028	2
Caesar & Loretz GmbH	Melatonina	21002239029	9
Caesar & Loretz GmbH	Melatonina	21002239030	3
Caesar & Loretz GmbH	Melatonina	21002239031	1
Caesar & Loretz GmbH	Melatonina	21002239034	2
Caesar & Loretz GmbH	Melatonina	21002239035	1
Caesar & Loretz GmbH	Melatonina	21002239036	2
Caesar & Loretz GmbH	Melatonina	22003650001	2
Caesar & Loretz GmbH	Melatonina	22003650002	2
Caesar & Loretz Hild…	Melatonina	19128006191280009	1
Caesar & Loretz/Noweda	Melatonina	19128006	1
Caesar & Loretz/Noweda	Melatonina	20001543012	1
Caesar&Loretz GmbH	Melatonina	20001543007	1
Cealo/Gehe	Melatonina	10296624	1
Cealo	Melatonina	12321422	1
Cealo	Melatonina	20001543010	1
Cealo	Melatonina	21000597001	2
EuRho/Gehe	Melatonina	2110002-01	1
Euro OTC	Melatonina	120008	1
Euro OTC	Melatonina	12001	2
Euro OTC	Melatonina	120400302	1
Euro OTC	Melatonina	1204003-02	12
Euro OTC	Melatonina	1305029-01	8
Euro OTC	Melatonina	1407028-01	1
Euro OTC	Melatonina	1407028-02	3
Euro OTC	Melatonina	151004101	3
Euro OTC	Melatonina	1510041-01	7
Euro OTC	Melatonina	15254316	1
Euro OTC	Melatonina	161004001	1
Euro OTC	Melatonina	1610040-01	6
Euro OTC	Melatonina	1610040-02	5
Euro OTC	Melatonina	170007	1
Euro OTC	Melatonina	1709020-01	14
Euro OTC	Melatonina	170920-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Melatonina	17305106	1
Euro OTC	Melatonina	17I28-B04-360883	2
Euro OTC	Melatonina	180401501	1
Euro OTC	Melatonina	1804015-01	7
Euro OTC	Melatonina	1804015-02	1
Euro OTC	Melatonina	190603001	1
Euro OTC	Melatonina	1906030-01	13
Euro OTC	Melatonina	190903101	1
Euro OTC	Melatonina	1909031-01	2
Euro OTC	Melatonina	200202901	1
Euro OTC	Melatonina	2002029-01	26
Euro OTC	Melatonina	2101018	1
Euro OTC	Melatonina	2101018-01	7
Euro OTC	Melatonina	2106005	1
Euro OTC	Melatonina	2106005-01	5
Euro OTC	Melatonina	2110002-01	14
Euro OTC	Melatonina	71296	1
Fagron	Melatonina	11/26-N07	1
Fagron	Melatonina	11F09-N02	1
Fagron	Melatonina	120009	2
Fagron	Melatonina	12G19-N03	1
Fagron	Melatonina	12I28-B04-361873	1
Fagron	Melatonina	12K13-N02	1
Fagron	Melatonina	1305029-01	1
Fagron	Melatonina	13D12N10	1
Fagron	Melatonina	13D12-N10	2
Fagron	Melatonina	13e22-n12	1
Fagron	Melatonina	13E22N12	1
Fagron	Melatonina	13E22-N12	1
Fagron	Melatonina	13H21-N06	4
Fagron	Melatonina	13H21-N065x	1
Fagron	Melatonina	13H29-B03	1
Fagron	Melatonina	13H29-B03-291180	2
Fagron	Melatonina	14G18-B01-297242	1
Fagron	Melatonina	14G18-B01-297244	1
Fagron	Melatonina	14G18-B01-297245	1
Fagron	Melatonina	150002	1
Fagron	Melatonina	15C20-B01-306077	1
Fagron	Melatonina	15C20-B01-306078	3
Fagron	Melatonina	15C20-B01-308426	3
Fagron	Melatonina	15C20-B01-308427	5
Fagron	Melatonina	15C20-B01-308428	1
Fagron	Melatonina	15C20-B01-327131	1
Fagron	Melatonina	15G06-B03-315183	5
Fagron	Melatonina	15G06-B03-318398	1
Fagron	Melatonina	15G06-B03-321298	3
Fagron	Melatonina	15G06-B03-321299	5
Fagron	Melatonina	15G06-B03-323733	2
Fagron	Melatonina	16343702	1
Fagron	Melatonina	16343708	1
Fagron	Melatonina	16G06-B01-324743	2
Fagron	Melatonina	16G06-B01-327131	4
Fagron	Melatonina	16G06-B01-329142	4
Fagron	Melatonina	17/28-B04-344438	2
Fagron	Melatonina	17/28-B04-344439	1
Fagron	Melatonina	17/28-B04-344440	3
Fagron	Melatonina	17/28-B04-347315	1
Fagron	Melatonina	17/28-B04-348747	1
Fagron	Melatonina	17/28-B04-353566	1
Fagron	Melatonina	17/28-B04-359318	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Melatonina	170007	5
Fagron	Melatonina	17128-B04-344439	1
Fagron	Melatonina	17128-B04-355634	1
Fagron	Melatonina	17128B0436869	1
Fagron	Melatonina	1728B04347313	1
Fagron	Melatonina	1728B04360882	1
Fagron	Melatonina	17C22-B01-337089	3
Fagron	Melatonina	17C22-B01-337090	4
Fagron	Melatonina	17C22-B01-337091	2
Fagron	Melatonina	17I28	2
Fagron	Melatonina	17I28-B04	2
Fagron	Melatonina	17I28-B04-344439	5
Fagron	Melatonina	17I28-B04-344440	1
Fagron	Melatonina	17I28-B04-347314	1
Fagron	Melatonina	17I28-B04-348747	3
Fagron	Melatonina	17I28-B04-351312	2
Fagron	Melatonina	17I28-B04-352328	4
Fagron	Melatonina	17I28-B04-353566	4
Fagron	Melatonina	17I28-B04-355634	2
Fagron	Melatonina	17I28-B04-355635	1
Fagron	Melatonina	17I28-B04-356971	2
Fagron	Melatonina	17I28-B04-359317	2
Fagron	Melatonina	17I28-B04-359318	1
Fagron	Melatonina	17I28-B04-360883	2
Fagron	Melatonina	17I28-B04-361869	1
Fagron	Melatonina	17I28B04361873	1
Fagron	Melatonina	17I28-B04-361873	2
Fagron	Melatonina	17l28-B04	1
Fagron	Melatonina	17l28-B04-360883	1
Fagron	Melatonina	19002851	1
Fagron	Melatonina	19003987	1
Fagron	Melatonina	1906030-01	1
Fagron	Melatonina	191280006	1
Fagron	Melatonina	19K04-F01	1
Fagron	Melatonina	19K04-F01/370622	1
Fagron	Melatonina	19K04-F01-370622	6
Fagron	Melatonina	19K04-F01-370623	2
Fagron	Melatonina	20A31-F02	5
Fagron	Melatonina	20A31-F02-372822	2
Fagron	Melatonina	20A31-F02-372823	1
Fagron	Melatonina	20A31-F02-372824	5
Fagron	Melatonina	20A31-F02-373915	2
Fagron	Melatonina	20A31-F02-377485	1
Fagron	Melatonina	21/24-Bo1-215466	1
Fagron	Melatonina	21I24-B01-215466	1
Fagron	Melatonina	21I24-B01-215649	2
Fagron	Melatonina	21I24-BO1-215649	1
Fagron	Melatonina	22A12-B09	1
Fagron	Melatonina	22A12-B09-219594	2
Fagron	Melatonina	24E09-B01-237419	1
Fagron	Melatonina	24E09-B01-240405	1
Fagron	Melatonina	B01-2156409	1
Fagron	Melatonina	F01-3706202	1
Fargon GmbH & Co.KG	Melatonina	16G06-B01-324743	1
Fargon/AHD	Melatonina	17I28-B04-356971	1
Farmalabor / Farmalabor	Melatonina	P1201556-000	1
Farmalabor	Melatonina	P1800033-000	1
Farmalabor	Melatonina	R1804925	1
Fgron	Melatonina	12G19-N03	1
GEHE 22.03.2014	Melatonina	13167302	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe amax	Melatonina	1709020-01	1
Gehe	Melatonina	11/26-N07	1
Gehe	Melatonina	11L21-N04	1
Gehe	Melatonina	12G19-N03	2
Gehe	Melatonina	13D12-N10	1
Gehe	Melatonina	13E22-N12	1
Gehe	Melatonina	1510041-01	1
Gehe	Melatonina	15254324	1
GEHE	Melatonina	17I28-B04	1
GEHE	Melatonina	17I-28-B04	1
Gehe	Melatonina	18210311	1
Gehe	Melatonina	18210320	1
Gehe	Melatonina	19128003	5
gehe	Melatonina	21002239005	1
GEHE	Melatonina	21002239028	1
Gehe	Melatonina	21002239038	1
Gehe	Melatonina	21002239039	1
gepepharm	Melatonina	15G06-B03-315183	1
Ichthyol Gesellschaft	Melatonina	16343708	1
Inresa	Melatonina	110005	1
Jacoby Gatt-Koller	Melatonina	22J00616	1
Jenne	Melatonina	22003650002	1
Kehr	Melatonina	21002239038	1
Kehr	Melatonina	21002239039	3
Koisser	Melatonina	140202	2
KS Pharma	Melatonina	XPS130428	1
Noweda	Melatonina	18210304	1
Noweda	Melatonina	18210318	1
Noweda	Melatonina	21002239006	1
Otto Geilenkirchen Aachen	Melatonina	21002239013	2
Phoenix 03.04.2014	Melatonina	12J19-N02	1
PHOENIX 14.04.2014	Melatonina	13E22-N12	1
Phoenix/Caesar & Lor…	Melatonina	21002239028	1
Phoenix	Melatonina	15C20-B01	1
Phoenix	Melatonina	16266903	1
Phoenix	Melatonina	18210315	1
Phoenix	Melatonina	191421112	1
Phoenix	Melatonina	200480406	1
Phoenix	Melatonina	200811308	1
Phoenix	Melatonina	21002239038	1
Phoenix	Melatonina	3368	1
Phönix 02.01.15	Melatonina	13H21-N06	1
Phönix 02.01.2014	Melatonina	1204003-02	1
Phönix 19.02.2014	Melatonina	13167301	2
Phönix Gotha	Melatonina	19128005	1
Phönix	Melatonina	11267111	1
phönix	Melatonina	15254308	1
Phönix	Melatonina	17305115	1
Phönix	Melatonina	18210303	2
Phönix	Melatonina	APALC/MCT17030111	1
Sanacorp Verbund	Melatonina	20A31-F02-372823	1
Sanacorp WE: 17.0518…	Melatonina	1709020-01	1
Sanacorp	Melatonina		1
Sanacorp	Melatonina	11267119	1
sanacorp	Melatonina	14110320	1
Sanacorp	Melatonina	161004001	1
Sanacorp	Melatonina	161004002	1
Sanacorp	Melatonina	17I28-B04	3
Sanacorp	Melatonina	17I28-B04-360883	1
Sanacorp	Melatonina	18210318	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Melatonina	20001543007	1
Sanacorp	Melatonina	20001543012	1
Sanacorp	Melatonina	21002239036	1
Sanacorp	Melatonina	22003650005	1
Sanacorp	Melatonina	APALC/MLT/161101M	1
Sanacorp	Melatonina	APALC/MLT/170301M	2
Sanacorp	Melatonina	APALC/MLT/170901M	1
Sanacorp	Melatonina	APMLT170901M	1
Sanacorp	Melatonina	MLT/SEP/170901	1
Sanaorp	Melatonina	16343707	1
SWATI/Phoenix	Melatonina	2002029-01	1
WE Sanacorp 28.11..2...	Melatonina	15254324	1

- 234 372 spectra from 1515 *Apo-Ident* customers from a total of 48 917 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Melatonina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Melatonina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	640	0	152 322
Type B	0	1019	0	201 065
Type C	0	1666	29	234 372

The substance/substance group *Melatonina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0625 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4112 %)
Type C	100.0000 % (> 99.9007 %)	98.2891 % (> 98.1121 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20834	22237	28,07	237,22
20835	21618	9,69	203,32
20987	21618	5,84	205,92
21618	21618	0,00	208,16
22237	22237	0,00	206,80
22892	22237	3,53	208,65
22893	22237	5,22	210,25
23889	23889	0,00	206,00
24128	24128	0,00	206,60
25542	25542	0,00	211,37
26415	24128	9,02	204,84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mentol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20036-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mentol; Mentholum

Special notes

When selecting the *Mentol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mentol	11	18	422

Second-stage model

For differentiation of the substance/substance group *Mentol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mentol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	123,02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mentol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mentol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mentol	13377404	21443	60	20131212
Caelo	Mentol	181522	24233	40	20180625*
Caelo	Mentol	2000170	25217	40	20200608*
Euro OTC	Mentol	1403022-02	21601	45	20140408
Euro OTC	Mentol	1509045	21932	60	20151008*
Euro OTC	Mentol	1603024	22657	40	20160429*
Euro OTC	Mentol	1608012	22825	40	20160902*
Euro OTC	Mentol	2103009	25591	40	20210322*
Euro OTC	Mentol	2204013	26091	40	20220517*
Euro OTC	Mentol	2204013	26091SI	20	20220517*
Fagron	Mentol	16L20-T04-044769	23596	40	20170116
Fagron	Mentol	18L04-T06-065445	24690	40	20181217

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 505 spectra of 12 reference samples from the substance/substance group *Mentol*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 457 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 805 spectra of 21 reference samples from the substance/substance group *Mentol*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mentol	160956	22452	60
Caelo	Mentol	170927	23312	40
Caelo	Mentol	171889	23668	40
Caelo	Mentol	183286	24666	40
Caelo	Mentol	192453	24877	40
Caelo	Mentol	20003371	25617	40
Caelo	Mentol	21000696	25655	40
Caelo	Mentol	22000117	26019	40
Caelo	Mentol	23003505	27131	40
Euro OTC	Mentol	1701014	23005	40
Euro OTC	Mentol	1705022	23427	40
Euro OTC	Mentol	1802003	23951	40
Euro OTC	Mentol	1905013	24599	40
Euro OTC	Mentol	1912006	25089	40
Euro OTC	Mentol	2009021	25425	40
Euro OTC	Mentol	2301002	26515	40
Euro OTC	Mentol	2307028	26869	40
Fagron	Mentol	22L03-B08-227346	26537	40
Caelo	Mentol	170927	23645	40
Caelo	Mentol	22000117	26019SI	10
Euro OTC	Mentol	1403022-02	21601†	15

- 201 279 spectra from a total of 4026 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2431 spectra from 1049 *Apo-Ident* customers from 434 batches from the substance/substance group *Mentol*.
- Among them are spectra of independent samples from 422 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Mentol	1187170	1
	Mentol	1291910	1
	Mentol	21000696016	1
	Mentol	21000696018	1
	Mentol	21000730009	1
	Mentol	21000730016	2
	Mentol	2103009-01	1
	Mentol	220003309003	1
	Mentol	22002585003	6
	Mentol	22003309002	1
	Mentol	22003309003	10
	Mentol	22003309005	2
	Mentol	22003309007	5
	Mentol	22003309012	1
	Mentol	2204013-01	4
	Mentol	2204013-02	1
	Mentol	22A14-B05-219347	4
	Mentol	22F02-B11	1
	Mentol	22F02-B11-222586	7
	Mentol	22F02-B11-22586	1
	Mentol	22F02-B11-222586	1
	Mentol	2301002-01	18
	Mentol	2301002-02	7
	Mentol	2307028-01	3
	Mentol	23B14-B26-227532	6
	Mentol	B03-2193406	1
08639701	Mentol	2301002-01	1
11,22	Mentol	21C12-B03-211790	1
AHC	Mentol	22F02-B11-222586	1
AHD	Mentol	1305010-01	1
AHD	Mentol	18128014	1
AHD	Mentol	21000696018	1
AHD	Mentol	23G19-B06-231924	1
Alliance Health 14.04..14	Mentol	1305010-02	1
Alliance Healthcare	Mentol	15363804	1
Alliance Healthcare	Mentol	19162801	1
Alliance Healthcare	Mentol	23G19-B06-231924	1
alliance	Mentol	21000730009	1
Andreas Imhof	Mentol	8052015	1
Anzag	Mentol	12/19-N10	1
Anzag	Mentol	16L20-T04-044769	1
Apo-ident	Mentol	1509045-03	1
apo-ident	Mentol	1705022-01	1
apoident	Mentol	1807044-01	1
Audor Pharma	Mentol	200902102	1
beyvers	Mentol	16095613	1
Bombastus	Mentol	16095620	1
Bombastus	Mentol	16L20-T04-053177	1

continued on the next page

Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caeelo/Noweda	Mentol	20000970006	1
Caele	Mentol	2004420002	1
Caelo	Mentol		4
Caelo	Mentol	1/AD1	1
Caelo	Mentol	10008029-02	1
Caelo	Mentol	10157615	1
Caelo	Mentol	1046973	2
Caelo	Mentol	1087209	1
Caelo	Mentol	11091405	1
Caelo	Mentol	1115262	2
Caelo	Mentol	1119I-01855	1
Caelo	Mentol	11202901	1
Caelo	Mentol	11202910	5
Caelo	Mentol	12020402	5
Caelo	Mentol	1202041	1
Caelo	Mentol	12020410	1
Caelo	Mentol	12020411	8
Caelo	Mentol	1204036-01	1
Caelo	Mentol	12246203	1
Caelo	Mentol	12246204	1
Caelo	Mentol	12246205	8
Caelo	Mentol	12246211	3
Caelo	Mentol	130501001	1
Caelo	Mentol	13102001	1
Caelo	Mentol	13103802	1
Caelo	Mentol	13103901	24
Caelo	Mentol	13159104	4
Caelo	Mentol	13159105	20
Caelo	Mentol	13159110	2
Caelo	Mentol	1320260	2
Caelo	Mentol	13377402	3
Caelo	Mentol	13377404	17
Caelo	Mentol	13377407	2
Caelo	Mentol	13377408	2
Caelo	Mentol	13377409	9
Caelo	Mentol	133774112	1
Caelo	Mentol	13377412	3
Caelo	Mentol	13377413	1
Caelo	Mentol	13D1N09	1
Caelo	Mentol	13G09-N09	1
Caelo	Mentol	1403022-01	1
Caelo	Mentol	1403022-02	1
Caelo	Mentol	1410004-01	2
Caelo	Mentol	1410004-02	2
Caelo	Mentol	14183004	14
Caelo	Mentol	14183006	1
Caelo	Mentol	14183008	3
Caelo	Mentol	14183011	2
Caelo	Mentol	14183012	3
Caelo	Mentol	14183014	2
Caelo	Mentol	14183017	3
Caelo	Mentol	14183020	1
Caelo	Mentol	1507601	1
Caelo	Mentol	15076101	8
Caelo	Mentol	15076104	1
Caelo	Mentol	15076106	12
Caelo	Mentol	15076112	10
Caelo	Mentol	15076113	9
Caelo	Mentol	15076115	3
Caelo	Mentol	15076118	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mentol	15076215	1
Caelo	Mentol	15076219	1
Caelo	Mentol	1509045-03	1
Caelo	Mentol	15286201	1
Caelo	Mentol	15286205	1
Caelo	Mentol	15286209	1
Caelo	Mentol	15286212	2
Caelo	Mentol	15286216	1
Caelo	Mentol	15363803	2
Caelo	Mentol	15363804	11
Caelo	Mentol	15363805	11
Caelo	Mentol	15363809	8
Caelo	Mentol	15363810	13
Caelo	Mentol	15363815	16
Caelo	Mentol	1536815	1
Caelo	Mentol	1603024-01	3
Caelo	Mentol	160719M	1
Caelo	Mentol	1608012-01	2
Caelo	Mentol	1608012-02	4
Caelo	Mentol	16081805	1
Caelo	Mentol	160956	1
Caelo	Mentol	16095601	1
Caelo	Mentol	16095602	3
Caelo	Mentol	16095603	5
Caelo	Mentol	16095604	1
Caelo	Mentol	16095606	17
Caelo	Mentol	16095609	1
Caelo	Mentol	16095613	13
Caelo	Mentol	16095614	16
Caelo	Mentol	16095616	1
Caelo	Mentol	16095617	2
Caelo	Mentol	16095619	17
Caelo	Mentol	16095620	9
Caelo	Mentol	160956217188904	1
Caelo	Mentol	16095625	2
Caelo	Mentol	16098614	1
Caelo	Mentol	161202M/15076111	1
Caelo	Mentol	16L20-T04-053177	1
Caelo	Mentol	1701014-01	3
Caelo	Mentol	170101402	1
Caelo	Mentol	1701014-02	2
Caelo	Mentol	170502201	1
Caelo	Mentol	1705022-01	9
Caelo	Mentol	17072001	1
Caelo	Mentol	17078004	2
Caelo	Mentol	17078006	2
Caelo	Mentol	17078009	1
Caelo	Mentol	170822M/16095616	1
Caelo	Mentol	17188903	25
Caelo	Mentol	171889035483	1
Caelo	Mentol	17188904	24
Caelo	Mentol	17188906	4
Caelo	Mentol	17328803	5
Caelo	Mentol	17328804	19
Caelo	Mentol	17351501	2
Caelo	Mentol	17351505	7
Caelo	Mentol	17351506	1
Caelo	Mentol	1738804	1
Caelo	Mentol	1802003-01	3
Caelo	Mentol	18128007	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mentol	18128008	7
Caelo	Mentol	18128009	19
Caelo	Mentol	18128012	1
Caelo	Mentol	18128014	1
Caelo	Mentol	18128015	20
Caelo	Mentol	18128015P-190718-7	1
Caelo	Mentol	18152202	4
Caelo	Mentol	18152205	5
Caelo	Mentol	18152210	2
Caelo	Mentol	18152214	2
Caelo	Mentol	18152216	2
Caelo	Mentol	1832605	1
Caelo	Mentol	18326805	1
Caelo	Mentol	18328601	3
Caelo	Mentol	18328604	2
Caelo	Mentol	18328605	31
Caelo	Mentol	18328610	3
Caelo	Mentol	18328611	1
Caelo	Mentol	18328612	28
Caelo	Mentol	1838605	1
Caelo	Mentol	18L04-T06-065445	2
Caelo	Mentol	190501301	1
Caelo	Mentol	190513-02	1
Caelo	Mentol	19051401	1
Caelo	Mentol	19091805	1
Caelo	Mentol	19162801	6
Caelo	Mentol	19245006	1
Caelo	Mentol	1924530006	1
Caelo	Mentol	192453004	1
Caelo	Mentol	192453006	24
Caelo	Mentol	192977003	2
Caelo	Mentol	192977004	8
Caelo	Mentol	20000970006	4
Caelo	Mentol	20001704005	3
Caelo	Mentol	20004049004	5
Caelo	Mentol	20004049007	3
Caelo	Mentol	20004420002	19
Caelo	Mentol	20004420003	1
Caelo	Mentol	2000442002	3
Caelo	Mentol	20044200002	1
Caelo	Mentol	20200712-2	1
Caelo	Mentol	20E22-B02-2025100	1
Caelo	Mentol	21000696007	1
Caelo	Mentol	21000696010	6
Caelo	Mentol	210006960100	1
Caelo	Mentol	21000696012	9
Caelo	Mentol	21000696015	5
Caelo	Mentol	21000696016	2
Caelo	Mentol	21000696017	1
Caelo	Mentol	21000730002	1
Caelo	Mentol	21000730003	19
Caelo	Mentol	21000730006	1
Caelo	Mentol	21000730007	1
Caelo	Mentol	21000730009	6
Caelo	Mentol	21000730010	1
Caelo	Mentol	21000730011	12
Caelo	Mentol	21000730012	1
Caelo	Mentol	21000730016	6
Caelo	Mentol	2100073011	1
Caelo	Mentol	2100080011	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mentol	2100096015	1
Caelo	Mentol	2100696007	1
Caelo	Mentol	211227(21000730003)	1
Caelo	Mentol	21C12-B03-211790	1
Caelo	Mentol	21C12-B03-2117900	1
Caelo	Mentol	22003309003	1
Caelo	Mentol	22003309004	2
Caelo	Mentol	2204013-01	1
Caelo	Mentol	22042002	1
Caelo	Mentol	220622(21000730009)	1
Caelo	Mentol	2416	1
Caelo	Mentol	25041402	1
Caelo	Mentol	25051301	1
Caelo	Mentol	2912110З	1
Caelo	Mentol	314Q01855	1
Caelo	Mentol	3912A-01855	1
Caelo	Mentol	4137664	1
Caelo	Mentol	5117A-01855	1
Caelo	Mentol	515M-01855	1
Caelo	Mentol	5315I-01855	1
Caelo	Mentol	617E-01855	1
Caelo	Mentol	62470307	1
Caelo	Mentol	687711	1
Caelo	Mentol	7111201	1
Caelo	Mentol	72173258	1
Caelo	Mentol	750137	1
Caelo	Mentol	814A-01855	1
Caelo	Mentol	90(17328804)	1
Caelo	Mentol	91(18128009)	1
Caelo	Mentol	92(18128015)	1
Caelo	Mentol	930716	1
Caelo	Mentol	97(192453006)	1
Caelo	Mentol	98(20004420002)	1
Caelo	Mentol	AP210305-02	1
Caelo	Mentol	IntCh311052	1
Caeolo/Gehe	Mentol	16096619	1
Caesar & Lorenz GmbH	Mentol	15076101	1
Caesar & Loretz GmbH…	Mentol	20004049007	1
Caesar & Loretz GmbH…	Mentol	21000696010	1
Caesar & Loretz GmbH…	Mentol	21000730009	2
Caesar & Loretz GmbH…	Mentol	11202910	1
Caesar & Loretz GmbH…	Mentol	12020402	1
Caesar & Loretz GmbH…	Mentol	12020411	1
Caesar & Loretz GmbH…	Mentol	13103901	1
Caesar & Loretz GmbH…	Mentol	18128009	1
Caesar & Loretz GmbH…	Mentol	18328605	1
Caesar & Loretz GmbH…	Mentol	1912006-01	3
Caesar & Loretz GmbH/A	Mentol	21003010002	1
Caesar & Loretz GmbH/AHD	Mentol	192453006	2
Caesar & Loretz GmbH/AHD	Mentol	21000730003	1
Caesar & Loretz GmbH…	Mentol	20004420002	1
Caesar & Loretz GmbH…	Mentol	18328612	2
Caesar & Loretz GmbH…	Mentol	20004420002	1
Caesar & Loretz GmbH…	Mentol	21000730011	1
Caesar & Loretz GmbH/G	Mentol	20004049007	1
Caesar & Loretz GmbH/Gehe	Mentol	18128015	1
Caesar & Loretz GmbH/Gehe	Mentol	191628	1
Caesar & Loretz GmbH/Gehe	Mentol	20004049007	1
Caesar & Loretz GmbH/Gehe	Mentol	21000696010	1
Caesar & Loretz GmbH/Gehe	Mentol	21000730016	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Mentol	18328605	1
Caesar & Loretz GmbH...	Mentol	22002585003	1
Caesar & Loretz GmbH...	Mentol	AP220321-05	1
Caesar & Loretz GmbH/Nowe	Mentol	20001704005	1
Caesar & Loretz GmbH...	Mentol	18152202	1
Caesar & Loretz GmbH...	Mentol	18328605	3
Caesar & Loretz GmbH...	Mentol	21000730003	1
Caesar & Loretz GmbH...	Mentol	192453006	1
Caesar & Loretz GmbH...	Mentol	20000970006	1
Caesar & Loretz GmbH...	Mentol	20004049004	1
Caesar & Loretz GmbH...	Mentol	192977004	1
Caesar & Loretz GmbH...	Mentol	192453006	1
Caesar & Loretz GmbH...	Mentol	20004420002	1
Caesar & Loretz GmbH...	Mentol	21000696012	1
Caesar & Loretz GmbH...	Mentol	21000730003	1
Caesar & Loretz GmbH...	Mentol	22003309003	1
Caesar & Loretz GmbH/Sana	Mentol	20000970006	1
Caesar & Loretz GmbH...	Mentol	17328804	1
Caesar & Loretz GmbH...	Mentol	192453006	1
Caesar & Loretz GmbH...	Mentol	20004049004	1
Caesar & Loretz GmbH...	Mentol	21000730006	1
Caesar & Loretz GmbH...	Mentol	21000730016	1
Caesar & Loretz GmbH...	Mentol	AP210401-02	1
Caesar & Loretz GmbH	Mentol	17328804	1
Caesar & Loretz GmbH	Mentol	18128007	2
Caesar & Loretz GmbH	Mentol	18128009	5
Caesar & Loretz GmbH	Mentol	18128015	2
Caesar & Loretz GmbH	Mentol	18152210	1
Caesar & Loretz GmbH	Mentol	183286001	3
Caesar & Loretz GmbH	Mentol	18328603	2
Caesar & Loretz GmbH	Mentol	18328604	3
Caesar & Loretz GmbH	Mentol	18328605	7
Caesar & Loretz GmbH	Mentol	18328610	1
Caesar & Loretz GmbH	Mentol	18328611	1
Caesar & Loretz GmbH	Mentol	18328612	7
Caesar & Loretz GmbH	Mentol	1905013-01	1
Caesar & Loretz GmbH	Mentol	19162801	2
Caesar & Loretz GmbH	Mentol	192453004	3
Caesar & Loretz GmbH	Mentol	192453006	8
Caesar & Loretz GmbH	Mentol	192453008	1
Caesar & Loretz GmbH	Mentol	192977004	4
Caesar & Loretz GmbH	Mentol	20000970007	1
Caesar & Loretz GmbH	Mentol	20001704005	2
Caesar & Loretz GmbH	Mentol	20004049004	1
Caesar & Loretz GmbH	Mentol	20004049007	4
Caesar & Loretz GmbH	Mentol	20004420001	1
Caesar & Loretz GmbH	Mentol	20004420002	14
Caesar & Loretz GmbH	Mentol	20004420003	1
Caesar & Loretz GmbH	Mentol	21000696010	1
Caesar & Loretz GmbH	Mentol	21000696012	1
Caesar & Loretz GmbH	Mentol	21000730002	1
Caesar & Loretz GmbH	Mentol	21000730003	8
Caesar & Loretz GmbH	Mentol	21000730009	5
Caesar & Loretz GmbH	Mentol	21000730010	1
Caesar & Loretz GmbH	Mentol	21000730011	5
Caesar & Loretz GmbH	Mentol	21000730016	4
Caesar & Loretz	Mentol	15363809	1
Caesar & Loretz	Mentol	18128007	1
Caesar&Lorenz	Mentol	21000696007	1
Caesar&Loretz GmbH	Mentol	21000730003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar&Loretz,Phönix	Mentol	15076106	1
Caesar/Noweda	Mentol	12020403	1
Caesar/Noweda	Mentol	12246211	1
Caesar/Noweda	Mentol	15076111	2
Cealo	Mentol	1705022-01	1
Celo/AHD	Mentol	16095620	1
Defektur	Mentol	18328612	1
E Plus	Mentol	1705022-01	1
Eur Rho	Mentol	1912006-01	1
EuRho/ Gehe	Mentol	1807044-01	1
EuRho/ Noweda	Mentol	2009021-01	1
EuRho/Alliance	Mentol	1701014-01	1
EuRho/Alliance	Mentol	1905013-02	1
EuRho/Fiebig	Mentol	1905013-01	1
EuRho/Fiebig	Mentol	2103009-02	1
EuRho/Gehe	Mentol	1807044-01	1
EuRho/Jenne	Mentol	180704401	1
EuRho/Jenne	Mentol	2103009-01euri	1
EuRho/Phönix	Mentol	1146105	1
Eurho/Phönix	Mentol	2009021-01	1
Eurho/Sanacorp	Mentol	1802003-01	1
EuRho/sanacorp	Mentol	1905013-01	1
EuRho	Mentol	1046973	1
EuRho	Mentol	1204036-02	1
EuRho	Mentol	1305010-01	1
EuRho	Mentol	1603024-01	1
EuRho	Mentol	1701014-02	1
Eurho	Mentol	170502201	1
EuRho	Mentol	1705022-01	2
EuRho	Mentol	1905013-01	1
EuRho	Mentol	1912006-01	1
euRho	Mentol	200902101	1
EuRho	Mentol	2103009-03	1
EuRho	Mentol	2910A-01855	1
EuRho	Mentol	915A-01855	1
Eurho-Phönix	Mentol	2204013-01	1
Euro OTC	Mentol	1001505	3
Euro OTC	Mentol	1001506	1
Euro OTC	Mentol	1002019-03	1
Euro OTC	Mentol	1008029-01	1
Euro OTC	Mentol	1046973	1
Euro OTC	Mentol	1087209	1
Euro OTC	Mentol	1105028-01	1
Euro OTC	Mentol	1111020-01	1
Euro OTC	Mentol	1146105	6
Euro OTC	Mentol	1178546	2
Euro OTC	Mentol	1201416	1
Euro OTC	Mentol	1204036-01	8
Euro OTC	Mentol	120403602	1
Euro OTC	Mentol	1204036-02	3
Euro OTC	Mentol	120-4036-02	2
Euro OTC	Mentol	1204036-1	1
Euro OTC	Mentol	1210017-01	4
Euro OTC	Mentol	1210017-02	12
Euro OTC	Mentol	1221331	5
Euro OTC	Mentol	130501001	1
Euro OTC	Mentol	1305010-01	7
Euro OTC	Mentol	130501002	1
Euro OTC	Mentol	1305010-02	6
Euro OTC	Mentol	1310J-01855	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Mentol	1337745	1
Euro OTC	Mentol	140302201	2
Euro OTC	Mentol	1403022-01	2
Euro OTC	Mentol	1403022-02	11
Euro OTC	Mentol	14030222-02	1
Euro OTC	Mentol	140322-01	1
Euro OTC	Mentol	141000401	1
Euro OTC	Mentol	1410004-01	21
Euro OTC	Mentol	1410004-02	12
Euro OTC	Mentol	14183012	1
Euro OTC	Mentol	15020006-02	1
Euro OTC	Mentol	1502006	1
Euro OTC	Mentol	150200601	1
Euro OTC	Mentol	1502006-01	18
Euro OTC	Mentol	1502006-02	17
Euro OTC	Mentol	1509045	2
Euro OTC	Mentol	1509045-01	4
Euro OTC	Mentol	150904502	1
Euro OTC	Mentol	1509045-02	11
Euro OTC	Mentol	15-0904502	1
Euro OTC	Mentol	1509045-03	15
Euro OTC	Mentol	1602024-01	1
Euro OTC	Mentol	1603021-01	1
Euro OTC	Mentol	1603024-01	46
Euro OTC	Mentol	160801201	2
Euro OTC	Mentol	1608012-01	25
Euro OTC	Mentol	1608012-02	14
Euro OTC	Mentol	1608012-1	1
Euro OTC	Mentol	1608012-12	1
Euro OTC	Mentol	16095614	1
Euro OTC	Mentol	16L20-T04-053177	1
Euro OTC	Mentol	1701014_01	1
Euro OTC	Mentol	17010140	1
Euro OTC	Mentol	170101401	1
Euro OTC	Mentol	1701014-01	20
Euro OTC	Mentol	170101402	4
Euro OTC	Mentol	1701014-02	23
Euro OTC	Mentol	1701014-2	1
Euro OTC	Mentol	170104-01	1
Euro OTC	Mentol	17050022-01	1
Euro OTC	Mentol	1705011-01	1
Euro OTC	Mentol	1705022	1
Euro OTC	Mentol	170502201	2
Euro OTC	Mentol	1705022-01	48
Euro OTC	Mentol	1705022011	1
Euro OTC	Mentol	1705022-1	1
Euro OTC	Mentol	1802003	1
Euro OTC	Mentol	1802003/01	1
Euro OTC	Mentol	180200301	4
Euro OTC	Mentol	1802003-01	59
Euro OTC	Mentol	1807044_01	1
Euro OTC	Mentol	180704401	1
Euro OTC	Mentol	1807044-01	44
Euro OTC	Mentol	180704402	1
Euro OTC	Mentol	1807044-02	5
Euro OTC	Mentol	18121718	1
Euro OTC	Mentol	182003-01	1
Euro OTC	Mentol	1905013	2
Euro OTC	Mentol	1905013_01	1
Euro OTC	Mentol	190501301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Mentol	1905013-01	29
Euro OTC	Mentol	1905013-02	17
Euro OTC	Mentol	1905013-023	1
Euro OTC	Mentol	191080810	1
Euro OTC	Mentol	1912006-01	47
Euro OTC	Mentol	1912006-1	1
Euro OTC	Mentol	195013-01	1
Euro OTC	Mentol	1987209	1
Euro OTC	Mentol	20009021	1
Euro OTC	Mentol	200902101	1
Euro OTC	Mentol	2009021-01	60
Euro OTC	Mentol	2009021-02	11
Euro OTC	Mentol	20116	1
Euro OTC	Mentol	2103009	1
Euro OTC	Mentol	210300901	5
Euro OTC	Mentol	2103009-01	41
Euro OTC	Mentol	2103009-02	11
Euro OTC	Mentol	2103009-03	14
Euro OTC	Mentol	2201013-01	1
Euro OTC	Mentol	220401301	1
Euro OTC	Mentol	2204013-01	14
Euro OTC	Mentol	2204013-02	5
Euro OTC	Mentol	2301002-01	5
Euro OTC	Mentol	25021709	1
Euro OTC	Mentol	5116U-01855	4
Euro OTC	Mentol	6102014B	1
Euro OTC	Mentol	696773	1
Euro OTC	Mentol	721123	1
Euro OTC	Mentol	807044-011	1
Euro OTC	Mentol	807862	1
Euro OTC	Mentol	858607	1
Euro OTC	Mentol	902-012	1
Euro OTC	Mentol	973192	3
Euro OTC	Mentol	B02-2025100	1
Euro OTC	Mentol	EN/20/01001	1
Euro OTC	Mentol	PM14	1
Euro Ph. / Gehe	Mentol	1701014-02	1
Euro/Jenne	Mentol	1807044-02	1
Euro/Phönix	Mentol	1905013-02	1
Euron	Mentol	1705022-01	1
Euron	Mentol	1905013-02	1
Euroo/Phönix	Mentol	210300901	1
Europharm	Mentol	130501-01	1
F/P	Mentol	20E22B022025010	1
Fagron	Mentol	1084145	1
Fagron	Mentol	1115262	4
Fagron	Mentol	11C01-N01	1
Fagron	Mentol	11G19-N07	1
Fagron	Mentol	12/19-N10	1
Fagron	Mentol	12/19-N100554/560	1
Fagron	Mentol	1201416	1
Fagron	Mentol	1219-N10	1
Fagron	Mentol	1247454	4
Fagron	Mentol	1289677	2
Fagron	Mentol	12C05-N03	1
Fagron	Mentol	12Cos-N03	1
Fagron	Mentol	12D23-N06	6
Fagron	Mentol	12F01-N14	3
Fagron	Mentol	12G20-N02	3
Fagron	Mentol	12I19-N10	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mentol	13D16-N09	7
Fagron	Mentol	13D16-N090631/1300	1
Fagron	Mentol	13G09-N09	1
Fagron	Mentol	13G09-N090204/520	1
Fagron	Mentol	13J21-N04	2
Fagron	Mentol	13O16-N09	1
Fagron	Mentol	14100041-01	1
Fagron	Mentol	14H29-M02	11
Fagron	Mentol	14H29-M04	1
Fagron	Mentol	15076101	1
Fagron	Mentol	15076115	1
Fagron	Mentol	1509045-03	1
Fagron	Mentol	16L20-T04	4
Fagron	Mentol	16L20-T04-044469	1
Fagron	Mentol	16L20T04044769	1
Fagron	Mentol	16L20-T04-044769	22
Fagron	Mentol	16l20T04-053177	1
Fagron	Mentol	16L20T04053177	1
Fagron	Mentol	16L20-T04-053177	13
Fagron	Mentol	16L20-To4	1
Fagron	Mentol	1701014-02	1
Fagron	Mentol	17o1014-02	1
Fagron	Mentol	1804T06065445	1
Fagron	Mentol	1807044-01	1
Fagron	Mentol	180L04-T06-065445	1
Fagron	Mentol	18204-T06	1
Fagron	Mentol	18G02T30	1
Fagron	Mentol	18G02-T30	3
Fagron	Mentol	18G02-T30-062159	26
Fagron	Mentol	18L04-T0-065445	1
Fagron	Mentol	18L04T06	1
Fagron	Mentol	18L04-T06	2
Fagron	Mentol	18L04-T06-065445	33
Fagron	Mentol	18l04-to6-065445	1
Fagron	Mentol	18L20-T04	1
Fagron	Mentol	18LO4-TO6-65445	1
Fagron	Mentol	20a31-b05-196609	1
Fagron	Mentol	20A31-b05-196609	1
Fagron	Mentol	20A31-B05-196609	15
Fagron	Mentol	20E22-B02202510	1
Fagron	Mentol	20E22-B02-202510	11
Fagron	Mentol	20e22-bo2-202510	1
Fagron	Mentol	21/13-B03-219346	2
Fagron	Mentol	2113-B03	1
Fagron	Mentol	2113B03219346	1
Fagron	Mentol	2113-BO3-219346	1
Fagron	Mentol	21C12-B03	3
Fagron	Mentol	21c12-b03-211790	1
Fagron	Mentol	21c12-B03-211790	1
Fagron	Mentol	21C12-B03-211790	19
Fagron	Mentol	21c12-bo3-211790	1
Fagron	Mentol	21C12-BO3-211790	1
Fagron	Mentol	21I13-B03	3
Fagron	Mentol	21I13-B03_219346	1
Fagron	Mentol	21I13-B03-219346	1
Fagron	Mentol	22A14-B05-219347	7
Fagron	Mentol	22F02-B11-222586	1
Fagron	Mentol	3-21934006	1
Fagron	Mentol	750137	1
Fagron	Mentol	778301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mentol	858607	1
Fagron	Mentol	976035	1
Fagron	Mentol	B02-2025100	1
Fagron	Mentol	B03-2117900	2
Fagron	Mentol	B03-2193406	5
Fargo/Gehe	Mentol	18G02-T30062159	1
Fargo/Gehe	Mentol	B03-2117900	1
Fargon/ Noweda	Mentol	13D16-N09	1
Fargon/GEHE	Mentol	18L04-T06-065445	1
Fargon	Mentol	18G02-T30-062159	1
Fargon	Mentol	18L04-T06-065445	1
Fargon	Mentol	20A31-B05-196609	1
Fargon	Mentol	B05-1966009	1
Fiebig	Mentol	16095625	1
Fiebig	Mentol	1705022-01	1
Fiebig	Mentol	17328803	1
Fiebig	Mentol	18L04-T06-065445	1
Finteler Apotheke	Mentol	16095614	1
Finze	Mentol	9221710	1
Fragon/Sanacorp	Mentol	16L20-T04-053177	1
Frey & Lau GmbH/Noweda	Mentol	1509045-03	2
Frey + Lau GmbH/AHD	Mentol	20A31-B05-196609	1
Frey + Lau GmbH	Mentol	21/13-B03-219346	1
Frey Lau GmbH	Mentol	1270077	2
Frey*Lau GmbH	Mentol	1305010-01	1
Frey*Lau GmbH	Mentol	973192	1
Frey+Lau GmbH / Noweda	Mentol	2009021-01	1
Frey+Lau GmbH Noweda	Mentol	1178546	1
Frey+Lau GmbH/Gehe	Mentol	1001505	1
Frey+Lau GmbH/Noweda	Mentol	1221331	1
Frey+Lau GmbH	Mentol	1178546	1
Frey+Lau GmbH	Mentol	1509045-02	1
Frey+Lau GmbH	Mentol	1603024-01	1
frey+Lau/jenne	Mentol	1087209	1
Frey+Lau	Mentol	926636	1
Gehe / Ensbona	Mentol	16L20-T04-044769	1
Gehe/ 27.10.12 EuRho	Mentol	11219216	1
Gehe	Mentol	12020411	1
Gehe	Mentol	13377412	1
Gehe	Mentol	13D16-N09	1
Gehe	Mentol	1502006-02	2
Gehe	Mentol	1608012-01	1
Gehe	Mentol	16095602	1
GEHE	Mentol	16L20-T04-044769	1
Gehe	Mentol	1705022-01	2
Gehe	Mentol	1802003-01	1
Gehe	Mentol	18128009	1
Gehe	Mentol	18128015	1
Gehe	Mentol	18G02-T30-062159	1
Gehe	Mentol	1905013-01	1
Gehe	Mentol	1905013-02	1
Gehe	Mentol	21000696012	1
Gehe	Mentol	2103009-01	1
Gehe	Mentol	22003309007	1
Gehe	Mentol	22A14-B05-219347	1
Gehe	Mentol	22F02-B11-222586	1
gehe	Mentol	2301002-02	1
Gehe	Mentol	2301002-02	1
GEHE	Mentol	B03-2193406	1
Geibo/Euro 24.1.17	Mentol	1608012-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
GUMO	Mentol	20004420002	1
Hageda	Mentol	20A31-B05-196609	1
Hedinger/Phönix	Mentol	17328802	1
Hepart	Mentol	1608012-02	1
Ichthyol / Phoenix	Mentol	16095603	1
Imhof	Mentol	15-5401	1
Jenne	Mentol	180200301	1
Kehr	Mentol	16095613	1
Kehr	Mentol	16095620	1
Kehr	Mentol	1802003-01	1
Kehr	Mentol	2204013-01	1
Kloster Apotheke	Mentol	9999999999	1
L10	Mentol	1705022-01	1
L12	Mentol	1603024-01	1
L12	Mentol	1802003-01	1
L12	Mentol	1807044-01	1
Menthol/Phoenix	Mentol	16L20-T04-044769	1
Nachprüfung	Mentol	123456	1
Nachprüfung	Mentol	28511041	1
Norex Flavours Pvt. ...	Mentol	15286205	2
Norex Flavours Pvt. ...	Mentol	15286207	1
Noweda	Mentol	1001505	1
Noweda	Mentol	1204036-01	1
Noweda	Mentol	1410004-01	1
Noweda	Mentol	15363809	1
Noweda	Mentol	1701014-02	1
Noweda	Mentol	1705022-01	1
Noweda	Mentol	17188904	1
Noweda	Mentol	1807044	1
Noweda	Mentol	180704401	1
Noweda	Mentol	1807044-01	1
Noweda	Mentol	1807044-02	1
Noweda	Mentol	1905013-01	1
Noweda	Mentol	20004049007	1
Noweda	Mentol	2009021	1
Noweda	Mentol	21000730011	2
Noweda	Mentol	2103009-02	1
Noweda	Mentol	21C12-B03	1
Noweda	Mentol	21C12-B03-211790	1
Noweda	Mentol	22002986002	1
NOWEDA	Mentol	2204013-01	1
Noweda	Mentol	22F02-B11-222586	2
Noweda	Mentol	2301002-01	2
Noweda	Mentol	2301002-02	1
Pala	Mentol	1802003-01	1
Ph.Eur.9.0	Mentol	1912006-01	1
Phoenix 15.04.2014	Mentol	12246211	1
Phoenix/Cealo	Mentol	1509045-01/4116F-018	1
Phoenix	Mentol	1146105	1
Phoenix	Mentol	1403022-02	1
Phoenix	Mentol	16095617	1
Phoenix	Mentol	16095619	1
Phoenix	Mentol	16095625	1
phoenix	Mentol	180704401	1
Phoenix	Mentol	1905013-01	1
Phoenix	Mentol	2204013-02	1
Phoenix	Mentol	2301002-01	1
PHOENIX	Mentol	2301002-02	1
Phoenix	Mentol	3127	1
Phoenix	Mentol	750137	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Mentol	B04-2029402	1
Phönix Gotha	Mentol	1410004-01	1
Phönix Gotha	Mentol	18L04-T06-065445	1
Phönix/EuRo	Mentol	2009021-01	1
Phönix	Mentol	12246204	1
Phönix	Mentol	13159105	1
phönix	Mentol	15363805	1
Phönix	Mentol	1608012-02	1
Phonix	Mentol	1802003-01	1
Phönix	Mentol	1802003-01	2
Phönix	Mentol	1807044-01	1
Phönix	Mentol	18128015	1
Phönix	Mentol	1905013-01	1
Phönix	Mentol	1912006-01	1
Phönix	Mentol	2009021-01	1
Phönix	Mentol	2103009-01	1
PHÖNIX	Mentol	21C12-B03-211790	1
Phönix	Mentol	22F02-B11-222586	2
Retest	Mentol	1305010-02	1
Sanacomp	Mentol	22003309003	1
Sanacorp Stralsund	Mentol	21C12-B03-211790	1
Sanacorp WE:02.09.16...	Mentol	15363809	1
Sanacorp	Mentol	1204036-01	1
Sanacorp	Mentol	1210017-01	1
Sanacorp	Mentol	1305010-01	1
Sanacorp	Mentol	13103901	1
Sanacorp	Mentol	13377409	1
Sanacorp	Mentol	16095613	1
Sanacorp	Mentol	16095619	1
Sanacorp	Mentol	17188903	1
Sanacorp	Mentol	17188904	1
Sanacorp	Mentol	17328804	1
Sanacorp	Mentol	18328605	1
Sanacorp	Mentol	18328612	1
Sanacorp	Mentol	1912006-01	1
Sanacorp	Mentol	20004420002	1
Sanacorp	Mentol	21000696016	1
Sanacorp	Mentol	21000730003	1
Sanacorp	Mentol	21000730011	1
Sanacorp	Mentol	2103009-02	1
sanacorp	Mentol	22003309003	1
Sanacorp	Mentol	22003309007	2
Sanacorp	Mentol	2204013-01	1
Sanacorp	Mentol	2301002-01	1
Sanacorp	Mentol	6/AKD3	1
siehe protokoll	Mentol	1008029-02	1
Spangro_12.03.2019	Mentol	1802003-01	1
VDL; 9.23EUR; 28.09.15	Mentol	15076113	1
WE:Sanacorp 03.11.20...	Mentol	15363810	1

- 233 636 spectra from 1515 *Apo-Ident* customers from a total of 48 835 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Mentol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mentol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	505	0	152 457
Type B	0	791	14	201 279
Type C	0	2425	6	233 636

The substance/substance group *Mentol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8119 %)
Type B	100.0000 % (> 99.9912 %)	98.2609 % (> 97.8882 %)
Type C	100.0000 % (> 99.9007 %)	99.7532 % (> 99.6298 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21443	22657	3,93	265,90
21601	21932	21,72	250,62
21932	21932	0,00	268,03
22657	22657	0,00	269,70
22825	22825	0,00	256,18
23596	22825	3,84	253,59
24233	24233	0,00	278,27
24690	22825	6,43	256,78
25217	25217	0,00	273,80
25591	25591	0,00	257,81
26091	26091	0,00	272,38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mesalazina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21772-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mesalazina; Mesalazinum

Special notes

When selecting the *Mesalazina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mesalazina	8	4	22

Second-stage model

For differentiation of the substance/substance group *Mesalazina* the following second-stage model is used:

- Submodelo 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mesalazina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	101,69	–
⋮	⋮	⋮
Clioquinol	>50	30,48
Ácido nicotínico	>50	32,83
Nitrato de miconazol	>50	43,94
Teofilina etilenodiamina hidratada	>50	156,73

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mesalazina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mesalazina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Mesalazina	1206029-04	21772	60	AR-15-FG-011819-01
Euro OTC	Mesalazina	1206029-04	21887	60	20140923
Euro OTC	Mesalazina	1602005	22518	40	20160218*
Euro OTC	Mesalazina	1602005-01	22925	40	20160218
Euro OTC	Mesalazina	1911016	25082	40	20191218*
Euro OTC	Mesalazina	2009037	25569	40	20210114*
Fagron	Mesalazina	15H13-B06-317177	22356	60	20150827
Fagron	Mesalazina	16I28-B02-327679	22929	40	20161128
Fagron	Mesalazina	22K26-B12-224459	26732	40	20230504
Fagron	Mesalazina	22K26-B12-224459	26732SI	20	20230504

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Mesalazina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 522 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Mesalazina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Mesalazina	1611019	22872	40
Euro OTC	Mesalazina	1902013	24477	40
Euro OTC	Mesalazina	2203020	26094	40
Fagron	Mesalazina	17A17-B03-336444	23934	40
Euro OTC	Mesalazina	2203020	26094SI	20

- 201 904 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 86 spectra from 14 *Apo-Ident* customers from 26 batches from the substance/substance group *Mesalazina*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Mesalazina	21F15-F50-382143	1
	Mesalazina	21J12-B18-216345	2
Caelo	Mesalazina	18C30-B05-353048	1
Euro OTC	Mesalazina		1
Euro OTC	Mesalazina	1206029-04	1
Euro OTC	Mesalazina	1602005-01	3
Euro OTC	Mesalazina	1602005-02	7
Euro OTC	Mesalazina	1611019-01	5
Euro OTC	Mesalazina	1611019-03	2
Euro OTC	Mesalazina	190201301	1
Euro OTC	Mesalazina	1902013-01	10
Euro OTC	Mesalazina	190213-01	1
Euro OTC	Mesalazina	1911016-01	3
Euro OTC	Mesalazina	2009037-01	4
Euro OTC	Mesalazina	200903702	1
Euro OTC	Mesalazina	2203020-01	2
Euro OTC	Mesalazina	B02-3638804	1
Fagron	Mesalazina		1
Fagron	Mesalazina	1100007129	1
Fagron	Mesalazina	16I28-B02-327679	24
Fagron	Mesalazina	18C30-B05-353048	4
Fagron	Mesalazina	19G05-B02-363884	1
Fagron	Mesalazina	20J13-F07-0374998	1
Fagron	Mesalazina	20J13-F07-374998	2
Fagron	Mesalazina	21F15-F02-379144	1
Fagron	Mesalazina	21F15-F02-379244	4
Fagron	Mesalazina	21F15-F02-382144	1

- 235 981 spectra from 1515 *Apo-Ident* customers from a total of 49 233 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mesalazina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mesalazina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	180	0	201 904
Type C	0	86	0	235 981

The substance/substance group *Mesalazina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.0233 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21772	21772	0,00	157,85
21887	21772	14,99	156,11
22356	22518	4,63	146,24
22518	22518	0,00	144,69
22925	22518	3,89	147,76
22929	22518	9,55	147,52
25082	25082	0,00	148,12
25569	25569	0,00	148,66
26732	22518	5,93	147,82

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metamizol sódico monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22634-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metamizol sódico monoidratado; Dipirona sódica monoidratada

Special notes

When selecting the *Metamizol sódico monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metamizol sódico monoidratado	5	3	5

Second-stage model

For differentiation of the substance/substance group *Metamizol sódico monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metamizol sódico monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	144,49	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metamizol sódico monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metamizol sódico monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metamizol sódico monoidratado	161610	22634	40	20160714*
Caelo	Metamizol sódico monoidratado	15362816	22666	40	20151106
Caelo	Metamizol sódico monoidratado	161610	23313	40	20160714*
Caelo	Metamizol sódico monoidratado	20001888002	25388	40	20200819
Caelo	Metamizol sódico monoidratado	22001474	26241	40	20220718*
Caelo	Metamizol sódico monoidratado	22001474	26241SI	20	20220718*
Caelo	Metamizol sódico monoidratado	23003148	27111	40	20240110*
Caelo	Metamizol sódico monoidratado	23003148	27111SI	20	20240110*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 8 reference samples from the substance/substance group *Metamizol sódico monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 682 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 130 spectra of 3 reference samples from the substance/substance group *Metamizol sódico monoidratado*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metamizol sódico monoidratado	15362815	22726	40
Caelo	Metamizol sódico monoidratado	170584	23924	40
Caelo	Metamizol sódico monoidratado	21002292003	25900	50

- 201 954 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Metamizol sódico monoidratado*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Metamizol sódico monoidratado	16161007	1
Caelo	Metamizol sódico monoidratado	17058404	6
Caelo	Metamizol sódico monoidratado	18026504	3
Caelo	Metamizol sódico monoidratado	20001888002	3
Caelo	Metamizol sódico monoidratado	21000105002	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metamizol sódico monoidratado	21002292003	2
Caesar & Loretz GmbH	Metamizol sódico monoidratado	21000105002	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metamizol sódico monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metamizol sódico monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	130	0	201 954
Type C	0	18	0	236 049

The substance/substance group *Metamizol sódico monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22634	22634	0,00	208,08
22666	27111	12,31	207,73
23313	23313	0,00	206,57
25388	23313	9,36	207,71
26241	26241	0,00	201,50
27111	27111	0,00	204,39

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metilcelulose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20705-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metilcelulose; Hidroxipropilcelulose; Hipromelose; HPMC; Hydroxypropylcellulosum; Methylcellulosum

Special notes

When selecting the *Metilcelulose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metilcelulose	24	16	251

Second-stage model

For differentiation of the substance/substance group *Metilcelulose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metilcelulose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	92,76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metilcelulose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metilcelulose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hidroxipropilcelulose	12093107	20686	40	1402049
Caelo	Hidroxipropilcelulose	14189804	21767	60	AR-15-FG-014922-01
Caelo	Hidroxipropilcelulose	15345001	22258	60	20151104
Caelo	Hidroxipropilcelulose	181146	24249	40	20180618*
Caelo	Hidroxipropilcelulose	20000942007	25426	40	20200505
Caelo	Hidroxipropilcelulose	21001994001	25981	40	20211004
Caelo	Hidroxipropilcelulose	21001994001	25981SI	30	20211004
Caelo	Hidroxipropilcelulose	22003732	26721	40	20230124*
Caelo	Hidroxipropilcelulose	22003732	26721SI	20	20230124*
Caelo	Hidroxipropilcelulose	24000194	27139	40	20240322*
Caelo	Hidroxipropilcelulose	24000194	27139SI	20	20240322*
Caelo	Hipromelose	13155006	20919	40	1402056
Caelo	Hipromelose	13155006	20931	40	20130529
Caelo	Hipromelose	14338801	21702	45	20141217
Caelo	Hipromelose	192852	25230	40	20191220*
Caelo	Hipromelose	20000987	25231	40	20200518*
Caelo	Hipromelose	21001141	26148	40	20210729*
Caelo	Hipromelose	22003524	26488	40	20221220*
Caelo	Hipromelose	22003524	26488SI	20	20221220*
Fagron	Hipromelose	15G08-B14-314845	22609	40	20150727
Fagron	Hipromelose	19G17-B04-194255	25060	40	20190830
Fagron	Hipromelose	22B26-B10-223114	26636	40	231005103

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metilcelulose	13130115	21570	60	20130517
Caelo	Metilcelulose	160602	22457	60	20160323*
Caelo	Metilcelulose	192473	25286	40	20191202*
Caelo	Metilcelulose	20002631	25622	40	20201027*
Fagron	Metilcelulose	12D02-N09	20705	40	1402447
Fagron	Metilcelulose	15H04-B07-331291	23224	40	20150824
Fagron	Metilcelulose	18D03-B05-361882	25188	40	20180507

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1175 spectra of 29 reference samples from the substance/substance group *Metilcelulose*. These samples are listed above in the *calibration samples* section. The reference samples come from 24 different batches.
- 151 787 spectra from a total of 2818 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 770 spectra of 21 reference samples from the substance/substance group *Metilcelulose*.
- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hidroxipropilcelulose	15345009	23123	40
Caelo	Hidroxipropilcelulose	17355801	23974	40
Caelo	Hipromelose	162244	22757	40
Caelo	Hipromelose	171150	23284	40
Caelo	Hipromelose	190696	24516	40
Caelo	Hipromelose	22001980	26242	40
Caelo	Hipromelose	23000497	26855	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hipromelose	24001679	27434	40
Caelo	Metilcelulose	171704	23627	40
Caelo	Metilcelulose	183318	24560	40
Caelo	Metilcelulose	22000891	26107	40
Caelo	Metilcelulose	23001536	26975	40
Caelo	Metilcelulose	24000306	27130	40
Fagron	Metilcelulose	20E28-F04-371902	25724	50
Fagron	Metilcelulose	21F04-F05-378883	25937	40
Fagron	Metilcelulose	22K07-B14-224511	26547	40
Caelo	Hipromelose	21001141	26148SI[†]	20
Caelo	Hipromelose	22001980	26242SI	20
Caelo	Metilcelulose	22000891	26107SI	20
Fagron	Metilcelulose	21F04-F05-378883	25937SI	40
Fagron	Metilcelulose	22K07-B14-224511	26547SI	20

- 201 314 spectra from a total of 4028 batches from further 840 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1216 spectra from 568 *Apo-Ident* customers from 266 batches from the substance/substance group *Metilcelulose*.
- Among them are spectra of independent samples from 250 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hipromelose	18004b03-348465	1
	Metilcelulose	22000891011	3
	Metilcelulose	22000891020	1
	Hipromelose	22003524002	3
	Hipromelose	22003524004	5
	Hipromelose	22003524005	1
	Hipromelose	22003524006	1
	Hipromelose	22003524007	3
	Hipromelose	23000497002	1
	Hipromelose	23000497003	10
	Metilcelulose	23001536003	2
	Hipromelose	23003602003	1
	Hipromelose	23D27-B06-227933	1
AHD	Hipromelose	16H23-B02-325994	1
AHD	Metilcelulose	192473004	1
AHD	Hipromelose	23000497003	2
Alliance Health 27.1...	Hipromelose	13D03-N03	1
Bombastus	Metilcelulose	17170405	1
Caelo	Metilcelulose		1
Caelo	Hipromelose	10004281003	1
Caelo	Metilcelulose	10247604	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metilcelulose	12044903	2
Caelo	Metilcelulose	12044907	1
Caelo	Metilcelulose	12044917	1
Caelo	Metilcelulose	12044918	2
Caelo	Metilcelulose	12044922	2
Caelo	Metilcelulose	12044927	6
Caelo	Metilcelulose	12044931	2
Caelo	Hipromelose	12098702	1
Caelo	Hipromelose	12215504	2
Caelo	Hipromelose	12215505	1
Caelo	Hipromelose	12239502	1
Caelo	Metilcelulose	13021401	1
Caelo	Hidroxipropilcelulose	13031306	1
Caelo	Hidroxipropilcelulose	13031309	1
Caelo	Hipromelose	13100304	2
Caelo	Metilcelulose	13130104	5
Caelo	Metilcelulose	13130109	5
Caelo	Metilcelulose	13130115	6
Caelo	Metilcelulose	13130121	3
Caelo	Metilcelulose	1313019	1
Caelo	Hipromelose	13155002	1
Caelo	Hipromelose	13155004	11
Caelo	Hipromelose	13d03-n03	1
Caelo	Hidroxipropilcelulose	14189801	2
Caelo	Metilcelulose	14197502	7
Caelo	Metilcelulose	14197513	1
Caelo	Metilcelulose	14197514	9
Caelo	Hipromelose	14338801	3
Caelo	Hipromelose	14338802	1
Caelo	Hipromelose	14338803	1
Caelo	Hipromelose	14C05-B03-294708	1
Caelo	Hidroxipropilcelulose	15129707	1
Caelo	Metilcelulose	15179602	12
Caelo	Metilcelulose	15179605	8
Caelo	Hidroxipropilcelulose	15345001	3
Caelo	Hidroxipropilcelulose	15345005	1
Caelo	Hidroxipropilcelulose	15345008	1
Caelo	Hipromelose	15B02-B05-308852	1
Caelo	Hipromelose	15G08-B14-310845	1
Caelo	Hipromelose	15G08-B14-314845	3
Caelo	Metilcelulose	16060202	1
Caelo	Metilcelulose	16060206	12
Caelo	Metilcelulose	16060210	12
Caelo	Hipromelose	16224401	6
Caelo	Hipromelose	16224403	15
Caelo	Hipromelose	16224404	1
Caelo	Hipromelose	16224406	5
Caelo	Hipromelose	16224407	19
Caelo	Hipromelose	16224408	1
Caelo	Hipromelose	16224409	11
Caelo	Metilcelulose	16284003	10
Caelo	Metilcelulose	16284004	2
Caelo	Metilcelulose	16284006	11
Caelo	Metilcelulose	1628404	1
Caelo	Hipromelose	16B16-B07-321327	2
Caelo	Hipromelose	16H23-B02-325994	1
Caelo	Hipromelose	16H23-B02-332066	1
Caelo	Hipromelose	17115004	2
Caelo	Hipromelose	17115005	22
Caelo	Hipromelose	17115008	13

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hipromelose	171150085501	1
Caelo	Hipromelose	17132101	1
Caelo	Metilcelulose	17170404	6
Caelo	Metilcelulose	17170405	11
Caelo	Metilcelulose	17170406	1
Caelo	Hipromelose	180215H/17115004	1
Caelo	Metilcelulose	18045101	11
Caelo	Metilcelulose	18045103	2
Caelo	Metilcelulose	18045107	2
Caelo	Metilcelulose	18045110	1
Caelo	Metilcelulose	18045114	3
Caelo	Hidroxipropilcelulose	18114601	1
Caelo	Hidroxipropilcelulose	18114607	2
Caelo	Hipromelose	18132101	16
Caelo	Hipromelose	18132102	6
Caelo	Hipromelose	18132105	21
Caelo	Hipromelose	18132106	2
Caelo	Hipromelose	18132109	13
Caelo	Hipromelose	18132111	6
Caelo	Hipromelose	18132111/18132109	1
Caelo	Hipromelose	18132116	1
Caelo	Metilcelulose	183318002	4
Caelo	Metilcelulose	18331803	10
Caelo	Metilcelulose	18331804	1
Caelo	Metilcelulose	18331806	20
Caelo	Hipromelose	18A17-B04-345100	1
Caelo	Hipromelose	18D04-B03-350745	2
Caelo	Hipromelose	18D04-B03-355144	1
Caelo	Hipromelose	1906901	1
Caelo	Hipromelose	1906908	1
Caelo	Hipromelose	19069601	37
Caelo	Hipromelose	19069608	19
Caelo	Hipromelose	19069609	9
Caelo	Metilcelulose	192473003	6
Caelo	Metilcelulose	192473004	6
Caelo	Hipromelose	192852004	4
Caelo	Hipromelose	192852005	27
Caelo	Hipromelose	19285205	1
Caelo	Hipromelose	1969609	1
Caelo	Hipromelose	19G17-B04-194255	1
Caelo	Hipromelose	200000987004	1
Caelo	Hipromelose	200000987006	1
Caelo	Hipromelose	20000987003	8
Caelo	Hipromelose	20000987004	24
Caelo	Hipromelose	20000987006	19
Caelo	Hipromelose	20000987007	5
Caelo	Hipromelose	20000987044	1
Caelo	Metilcelulose	200014546013	1
Caelo	Hipromelose	20004281002	4
Caelo	Hipromelose	20004281003	7
Caelo	Metilcelulose	20004546004	4
Caelo	Metilcelulose	20004546008	5
Caelo	Metilcelulose	20004546009	5
Caelo	Metilcelulose	20004546013	4
Caelo	Metilcelulose	2000456009	1
Caelo	Hipromelose	2001980005	1
Caelo	Metilcelulose	20021401	1
Caelo	Hipromelose	21001141001	2
Caelo	Hipromelose	21001141002	9
Caelo	Hipromelose	21001141004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hipromelose	21001141005	7
Caelo	Hipromelose	21001141006	8
Caelo	Hipromelose	21001141009	1
Caelo	Hipromelose	210011411005	1
Caelo	Hidroxipropilcelulose	21001994001	1
Caelo	Metilcelulose	22000891002	3
Caelo	Metilcelulose	22000891007	1
Caelo	Metilcelulose	22000891011	1
Caelo	Hipromelose	22001980004	2
Caelo	Hipromelose	22001980005	24
Caelo	Hipromelose	22001980009	1
Caelo	Hipromelose	22001982225	1
Caelo	Hipromelose	22003524004	3
Caelo	Hipromelose	22003524005	2
Caelo	Hipromelose	22003524006	1
Caelo	Hipromelose	22003524007	1
Caelo	Metilcelulose	5081404	1
Caelo	Hipromelose	5121818	1
Caelo	Metilcelulose	5219Q-01882	1
Caelo	Hipromelose	D180F8Q011	1
Caesar & Loretz GmbH...	Hipromelose	16224403	1
Caesar & Loretz GmbH...	Metilcelulose	18331803	1
Caesar & Loretz GmbH...	Metilcelulose	20004546008	1
Caesar & Loretz GmbH...	Hipromelose	20000987006	1
Caesar & Loretz GmbH...	Hipromelose	21001141005	1
Caesar & Loretz GmbH/AHD	Hipromelose	19069609	1
Caesar & Loretz GmbH/AHD	Hipromelose	192852005	3
Caesar & Loretz GmbH/AHD	Hipromelose	20000987004	2
Caesar & Loretz GmbH...	Metilcelulose	20004546004	1
Caesar & Loretz GmbH...	Hipromelose	19069601	1
Caesar & Loretz GmbH/Gehe	Hipromelose	19069601	2
Caesar & Loretz GmbH/Gehe	Hidroxipropilcelulose	20000942005	1
Caesar & Loretz GmbH/GEHE	Hidroxipropilcelulose	20000942005	1
Caesar & Loretz GmbH/Gehe	Hipromelose	20000987004	1
Caesar & Loretz GmbH/Gehe	Hipromelose	20004281003	1
Caesar & Loretz GmbH/Gehe	Metilcelulose	22000891002	2
Caesar & Loretz GmbH...	Metilcelulose	18331806	1
Caesar & Loretz GmbH...	Hipromelose	19069608	1
Caesar & Loretz GmbH...	Hipromelose	22001980004	1
Caesar & Loretz GmbH...	Hipromelose	22001980005	1
Caesar & Loretz GmbH...	Metilcelulose	17170405	1
Caesar & Loretz GmbH...	Hipromelose	19069601	1
Caesar & Loretz GmbH...	Hipromelose	19069609	2
Caesar & Loretz GmbH...	Hipromelose	21001141005	1
Caesar & Loretz GmbH...	Metilcelulose	20004546004	1
Caesar & Loretz GmbH/Ph	Hipromelose	19069608	4
Caesar & Loretz GmbH...	Hidroxipropilcelulose	20003818001	1
Caesar & Loretz GmbH/Sana	Hipromelose	21001141005	1
Caesar & Loretz GmbH...	Metilcelulose	18331806	1
Caesar & Loretz GmbH...	Hipromelose	19069601	1
Caesar & Loretz GmbH...	Hipromelose	20000987004	1
Caesar & Loretz GmbH...	Metilcelulose	20004546004	1
Caesar & Loretz GmbH...	Hipromelose	22001980009	1
Caesar & Loretz GmbH	Metilcelulose	12044922	1
Caesar & Loretz GmbH	Metilcelulose	18045107	1
Caesar & Loretz GmbH	Metilcelulose	18045114	2
Caesar & Loretz GmbH	Hidroxipropilcelulose	18114605	1
Caesar & Loretz GmbH	Hipromelose	18132105	1
Caesar & Loretz GmbH	Hipromelose	18132109	1
Caesar & Loretz GmbH	Hipromelose	18132111	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Metilcelulose	183318022	1
Caesar & Loretz GmbH	Metilcelulose	18331803	4
Caesar & Loretz GmbH	Metilcelulose	18331806	9
Caesar & Loretz GmbH	Hipromelose	19069601	9
Caesar & Loretz GmbH	Hipromelose	19069608	2
Caesar & Loretz GmbH	Hipromelose	19069609	1
Caesar & Loretz GmbH	Metilcelulose	192473003	4
Caesar & Loretz GmbH	Metilcelulose	192473004	7
Caesar & Loretz GmbH	Hipromelose	192852004	1
Caesar & Loretz GmbH	Hipromelose	192852005	7
Caesar & Loretz GmbH	Hidroxipropilcelulose	20000942007	2
Caesar & Loretz GmbH	Hipromelose	20000987003	1
Caesar & Loretz GmbH	Hipromelose	20000987004	2
Caesar & Loretz GmbH	Hipromelose	20000987006	3
Caesar & Loretz GmbH	Hipromelose	20004281002	1
Caesar & Loretz GmbH	Hipromelose	20004281003	6
Caesar & Loretz GmbH	Metilcelulose	20004546004	3
Caesar & Loretz GmbH	Metilcelulose	20004546008	4
Caesar & Loretz GmbH	Metilcelulose	20004546009	2
Caesar & Loretz GmbH	Metilcelulose	20004546013	3
Caesar & Loretz GmbH	Hipromelose	21001141002	7
Caesar & Loretz GmbH	Hipromelose	21001141004	1
Caesar & Loretz GmbH	Hipromelose	21001141005	7
Caesar & Loretz GmbH	Hipromelose	21001141006	8
Caesar & Loretz GmbH	Hipromelose	21001141009	2
Caesar & Loretz GmbH	Metilcelulose	22000891002	4
Caesar & Loretz GmbH	Metilcelulose	22000891011	1
Caesar & Loretz GmbH	Hipromelose	22001980004	2
Caesar & Loretz GmbH	Hipromelose	22001980005	8
Caesar & Loretz GmbH	Hipromelose	22001980009	2
Caesar & Loretz GmbH	Hipromelose	22003524005	2
CAESAR & LORETZ GMBH	Hipromelose	B02-1977101	1
Caesar & Loretz	Hipromelose	17115005	1
Caesar & Loretz	Hipromelose	17115008	1
Caesar & Loretz	Hipromelose	18132116	1
Caesar&Lorenz/AHD	Metilcelulose	18045107	1
Cealo / AHD 19.09.20...	Hipromelose	19069601	1
Cealo/Gehe	Hipromelose	18132101	1
cealo	Metilcelulose	15179602	1
Cealo	Hipromelose	192852004	1
DOW Chemical Company...	Hipromelose	14G02-B11-296850	1
DOW chemical Company...	Hipromelose	15G08-B14-310845	1
Euro OTC	Metilcelulose	10247609	1
Euro OTC	Metilcelulose	15179602	1
Euro OTC	Metilcelulose	16284003	1
Euro OTC	Hipromelose	18132105	1
Euro OTC	Metilcelulose	18331806	1
Euro OTC	Hipromelose	21001141002	1
Fagron	Hipromelose		1
Fagron	Hipromelose	10G09-N03	1
Fagron	Hipromelose	12A30-N02	3
Fagron	Hipromelose	12D03-N03	1
Fagron	Hipromelose	12E02-N03	3
Fagron	Hipromelose	12G23-N03	1
Fagron	Hipromelose	12G23-NO3	1
Fagron	Metilcelulose	12H06-N06	2
Fagron	Hipromelose	12H20-N05	1
Fagron	Metilcelulose	13/26-N04	1
Fagron	Metilcelulose	131301(09)	1
Fagron	Hipromelose	13D03N03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hipromelose	13D03-N03	7
Fagron	Metilcelulose	13E02-B03-290531	3
Fagron	Hipromelose	13E02-B03-290532	1
Fagron	Hipromelose	13h09-m04	1
Fagron	Hipromelose	13H09-N04	9
Fagron	Metilcelulose	14A28-B04-295982	1
Fagron	Hipromelose	14C05B03	1
Fagron	Hipromelose	14C05-B03	1
Fagron	Hipromelose	14C-05B03	1
Fagron	Hipromelose	14c05-B03-294708	1
Fagron	Hipromelose	14C05-B03-294708	4
Fagron	Hipromelose	14C05-B03-294711	1
Fagron	Hipromelose	14G02-B11	3
Fagron	Hipromelose	14G02-B11-296850	6
Fagron	Hipromelose	14G02-B11-296851	1
Fagron	Hipromelose	14g02-b11-302118	2
Fagron	Hipromelose	14G02-B11-302118	7
Fagron	Hipromelose	14G02-B11-302119	1
Fagron	Hipromelose	14G02-B11-302121	1
Fagron	Hipromelose	15B02-B05	1
Fagron	Hipromelose	15B02-B05-308852	1
Fagron	Hipromelose	15G08-B14	1
Fagron	Hipromelose	15g08-b14-310845	2
Fagron	Hipromelose	15G08-B14-310845	10
Fagron	Hipromelose	15G08B14314185	2
Fagron	Hipromelose	15g08-b14-314845	1
Fagron	Metilcelulose	15G08B14314845	1
Fagron	Hipromelose	15G08-B14-314845	7
Fagron	Hipromelose	16B16_B07	1
Fagron	Hipromelose	16B16-B07_321327	1
Fagron	Hipromelose	16B16-B07-318276	2
Fagron	Hipromelose	16b16-b07-318531	1
Fagron	Hipromelose	16B16-B07-318531	8
Fagron	Hipromelose	16B16-B07-321327	3
Fagron	Hipromelose	16B-16-B07-321327	1
Fagron	Hipromelose	16B16-B07-321328	1
Fagron	Hipromelose	16B16-B07-321579	1
Fagron	Hipromelose	16B16-B07-323114	3
Fagron	Hipromelose	16B16-B07-325280	7
Fagron	Hipromelose	16H23B-02	1
Fagron	Hipromelose	16H23-B02-325994	1
Fagron	Hipromelose	16H23-B02-332066	8
Fagron	Hipromelose	17115005	1
Fagron	Hipromelose	18A17-B04	2
Fagron	Hipromelose	18A17-B04-345100	5
Fagron	Hipromelose	18A17-B04-346208	1
Fagron	Hipromelose	18D04-B03	4
Fagron	Hipromelose	18D04-B03-348465	6
Fagron	Hipromelose	18D04-B03-350745	3
Fagron	Hipromelose	18D04-B03-35144	1
Fagron	Hipromelose	18D04-B03-352349	1
Fagron	Hipromelose	18D04-B03-352746	4
Fagron	Hipromelose	18D04-B03-355144	3
Fagron	Hipromelose	18G17-B04-194255	1
Fagron	Hipromelose	19G17-B04	5
Fagron	Hipromelose	19G17-B04-194255	5
Fagron	Hipromelose	19G17-B04-194735	3
Fagron	Hipromelose	1AO1012N11	1
Fagron	Hipromelose	1J31012N11	3
Fagron	Hipromelose	1KO1012N11	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hipromelose	20110612-2	1
Fagron	Hipromelose	20D22-B02	1
Fagron	Hipromelose	20D22-B02-197710	7
Fagron	Hipromelose	20D22-B02-1977101	1
Fagron	Hipromelose	20D22-B02-197711	4
Fagron	Hipromelose	20D2-B02-197710	1
Fagron	Hipromelose	20G14-B01	3
Fagron	Hipromelose	20G14-B01-201924	1
Fagron	Hipromelose	21B26-B07-218984	1
Fagron	Hipromelose	220401M	1
Fagron	Hipromelose	2818A-01860	1
Fagron	Hipromelose	2H12012N12	1
Fagron	Hipromelose	20d22-B02-197711	1
Fagron	Hipromelose	20D22-B02-197710	1
Fagron	Hipromelose	2x19G17-B04-194735	1
Fagron	Hipromelose	325994	1
Fagron	Hipromelose	349970	1
Fagron	Hipromelose	3G08012N11	1
Fagron	Hipromelose	615I-01860	1
Fagron	Hipromelose	700182-0001	2
Fagron	Hipromelose	9088155	3
Fagron	Hipromelose	B01-2019204	2
Fagron	Hipromelose	B02-1977100	2
Fagron	Hipromelose	B04-1942505	1
Fagron	Hipromelose	B97-2101203	1
Fagron	Hipromelose	D180F8Q011	1
Fagron	Hipromelose	D180HBA012	1
Fagron	Hipromelose	D180J45013	1
Fagron	Hipromelose	YI16012N11	1
Fagron	Hipromelose	ZH19012N12	1
Fargon/Gehe	Hipromelose	18D04-B03-352746	1
Fiebig	Metilcelulose	18045101	1
Fragon/Phoenix	Hipromelose	18D04-b03-349970	1
FRAGON/Poenix	Hipromelose	16B16-B07-18276	1
Gatt-Koller / Phoenix	Hipromelose	14C05-B03-291647	2
Gatt-Koller	Metilcelulose	18045107	1
Gehe / 26.10.12 Fragon	Hipromelose	9D30-N05	1
Gehe amax	Hipromelose	19G17-B04-194735	1
Gehe	Hipromelose	14G02-B11	1
Gehe	Hipromelose	15G08-B14-310845	1
Gehe	Metilcelulose	16284003	1
GEHE	Hipromelose	16H23-B02	1
GEHE	Hipromelose	17115008	1
GEHE	Hipromelose	18049201	1
GEHE	Hipromelose	18A17-B04	3
Gehe	Hipromelose	19069601	1
gehe	Hipromelose	192852004	1
Jenne	Hipromelose	15G08-B14	1
Jenne	Hipromelose	18D04-B03-350745	2
Jenne	Hipromelose	20G14-B01-201924	2
Jenne	Metilcelulose	21B26-B07-213871	1
Kehr	Hipromelose	17115005	1
L12	Hipromelose	16224406	1
L12	Metilcelulose	16284003	1
L12	Hipromelose	17115008	1
L12	Metilcelulose	17170405	1
Nachprüfung 2609	Hipromelose	11H26-N01	1
Nachprüfung	Hipromelose	3082019-3	1
Noweda	Hipromelose	1315505	1
Noweda	Hipromelose	17115008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Metilcelulose	17170405	1
Noweda	Hidroxipropilcelulose	18114605	1
Noweda	Hipromelose	18132111	1
Noweda	Metilcelulose	18331806	1
Noweda	Hipromelose	18D04-B03-355144	1
Noweda	Hipromelose	19069603	1
Noweda	Hipromelose	2003524007	1
Noweda	Hipromelose	22003524004	2
Noweda	Hipromelose	D180HBA012	1
Phoenix/Cealo	Metilcelulose	17170404	1
Phoenix	Hipromelose	13E02-B03	1
Phoenix	Hipromelose	14c05-b03-294708	1
Phoenix	Hipromelose	16224407	1
Phoenix	Hipromelose	16B16-B07	2
Phoenix	Hipromelose	16B16-B07-321327	1
Phoenix	Metilcelulose	18331803	1
Phoenix	Metilcelulose	23001536003	1
Phönix Gotha	Hipromelose	14G02-B11-296850	1
Phonix	Hipromelose	13H09-N04	1
Phönix	Hipromelose	16224403	1
PHÖNIX	Hipromelose	16H23-B02-325994	1
Phönix	Hipromelose	2000987004	1
Phönix	Hipromelose	23000497003	1
Sanacorp 08.11.21, 22,95EUR	Hipromelose	211125H	1
Sanacorp	Metilcelulose	1717405	1
Sanacorp	Metilcelulose	18331803	1
Sanacorp	Hipromelose	19069608	1
Sanacorp	Hipromelose	22001980005	2
Sanacorp	Hipromelose	23000497003	2
Sanacorp	Hipromelose	2H12012N12	1

- 234 851 spectra from 1515 *Apo-Ident* customers from a total of 48 997 batches from a further 719 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metilcelulose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metilcelulose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1175	0	151 787
Type B	0	770	0	201 314
Type C	0	1202	14	234 851

The substance/substance group *Metilcelulose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4894 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2208 %)
Type C	100.0000 % (> 99.9007 %)	98.8487 % (> 98.6020 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20686	20686	0,00	179,52
20705	20705	0,00	155,97
20919	20919	0,00	164,76
20931	20919	7,55	168,38
21570	22457	15,39	157,10
21702	20919	30,72	160,78
21767	21767	0,00	172,56
22258	21767	16,07	177,93
22457	22457	0,00	156,08
22609	26488	17,21	173,94
23224	22457	11,00	156,82
24249	24249	0,00	160,74
25060	26636	32,84	158,18
25188	22457	18,73	152,31
25230	25230	0,00	168,49
25231	25231	0,00	169,51
25286	25286	0,00	151,72
25426	21767	8,30	175,35
25622	25622	0,00	160,91
25981	21767	17,87	171,84
26148	26148	0,00	171,95
26488	26488	0,00	172,66
26636	26636	0,00	153,72
26721	26721	0,00	192,17
27139	27139	0,00	180,80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metilprednisolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20953-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metilprednisolona; Methylprednisolonum

Special notes

When selecting the *Metilprednisolona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metilprednisolona	4	4	3

Second-stage model

For differentiation of the substance/substance group *Metilprednisolona* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metilprednisolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	80,06	–
⋮	⋮	⋮
Prednisolona	>50	73,64
Tirotricina	>50	83,92
Betametasona	>50	87,57
Triancinolona acetonido	>50	94,52
Fluocinolona acetonida	>50	97,53
Gramicidina	>50	137,80
Dexametasona	>50	174,94

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metilprednisolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metilprednisolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Metilprednisolona	13G19-N05	20953	40	1402438
Fagron	Metilprednisolona	15I04-B05-311572	22275	45	AR-16-FG-009102-01
Fagron	Metilprednisolona	15I04-B05-311572	22275SI	45	AR-16-FG-009102-01
Fagron	Metilprednisolona	15I04-B05-311572	22354	45	20151026
Fagron	Metilprednisolona	15I04-B05-311572	22354SI	45	20151026
Fagron	Metilprednisolona	18E16-B02-B02-358166	24572	40	20180611
Fagron	Metilprednisolona	21C30-F03-377878	25725	50	20210505
Fagron	Metilprednisolona	21C30-F03-377878	25725SI	50	20210505

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Metilprednisolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 602 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 8 reference samples from the substance/substance group *Metilprednisolona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Metilprednisolona	12D17-N04	20650	40
Fagron	Metilprednisolona	15L15-B01-321887	23229	40
Fagron	Metilprednisolona	18A03-B05-345742	23997	40
Fagron	Metilprednisolona	22D14-B07-227694	26619	40
Fagron	Metilprednisolona	15L15-B01-321887	23229SI	30
Fagron	Metilprednisolona	18A03-B05-345742	23997SI	40
Fagron	Metilprednisolona	18E16-B02-B02-358166	24572SI†	40
Fagron	Metilprednisolona	22D14-B07-227694	26619SI	40

- 201 774 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Metilprednisolona*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Metilprednisolona	22D14-B07-221096	1
Fagron	Metilprednisolona	12D17-N04	1
Fagron	Metilprednisolona	18A03-B05	1

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metilprednisolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metilprednisolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	310	0	201 774
Type C	0	3	0	236 064

The substance/substance group *Metilprednisolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20953	20953	0,00	144,55
22275	22275	0,00	149,53
22354	22275	6,08	151,32
24572	22275	12,97	146,98
25725	22275	24,88	143,27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metionina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20971-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metionina

Special notes

When selecting the *Metionina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metionina	6	9	1

Second-stage model

For differentiation of the substance/substance group *Metionina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metionina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aspartato de ornitina	96,16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metionina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metionina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Metionina	1602012	22368	60	20160219*
Euro OTC	Metionina	2011016	25469	40	20201130*
Euro OTC	Metionina	2108013	25763	50	20210902*
Fagron	Metionina	12K01-N03	20971	40	1402432
Fagron	Metionina	13L19-B36-295115	21786	60	20140108
Fagron	Metionina	19L20-F03-370997	25747	50	20200213

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 6 reference samples from the substance/substance group *Metionina*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 662 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 410 spectra of 12 reference samples from the substance/substance group *Metionina*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Metionina	1609024	22787	40
Euro OTC	Metionina	1703042	23126	40
Euro OTC	Metionina	1710008	23777	40
Euro OTC	Metionina	1904012	24674	40
Euro OTC	Metionina	1909004	24851	40
Euro OTC	Metionina	2205001	26194	40
Euro OTC	Metionina	2301004	26529	40
Euro OTC	Metionina	2305026	26769	30
Fagron	Metionina	23A16-B02-226111	26635	40
Euro OTC	Metionina	2205001	26194SI	20
Euro OTC	Metionina	2301004	26529SI	20
Fagron	Metionina	23A16-B02-226111	26635SI	20

- 201 674 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Metionina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Metionina	21A08-F04-376464	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metionina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metionina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	410	0	201 674
Type C	0	1	0	236 066

The substance/substance group *Metionina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5366 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20971	20971	0,00	189,65
21786	22368	7,53	188,60
22368	22368	0,00	190,99
25469	25469	0,00	190,24
25747	25763	11,04	189,07
25763	25763	0,00	189,75

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metoxisaleno**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20233-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metoxisaleno; Methoxsalenum

Special notes

When selecting the *Metoxisaleno* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metoxisaleno	8	11	106

Second-stage model

For differentiation of the substance/substance group *Metoxisaleno* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metoxisaleno* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	123,60	–
⋮	⋮	⋮
Cloridrato de ciprofloxacina	>50	279,44
Citrato de sódio	>50	285,81
Capsaicina	>50	330,66
Prednicarbato	>50	341,86
Levocarnitina	>50	353,46
Cloridrato de quinina di-hidratado	>50	371,98
Cloridrato de oxibutinina	>50	383,04
Acetato de ciproterona	>50	427,61
Triclosan	>50	439,07
Piridoxal-5-fosfato	>50	465,80
Heparina sódica	>50	674,37
Tetracaína	>50	691,06
Cloridrato de amitriptilina	>50	898,43
Alfaestradiol	>50	956,29
Valina	>50	998,36
Acetato de noretisterona	>50	1316,79
Sacarose	>50	2025,22
Amifampridina	>50	2149,98

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metoxisaleno* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metoxisaleno*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metoxisaleno	16103003	23167	40	20160415
Caelo	Metoxisaleno	170781	23333	40	20170427*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metoxisaleno	170781	23346	40	20170427*
Euro OTC	Metoxisaleno	130604101	21555	60	20130805
Euro OTC	Metoxisaleno	1506013	21862	60	20150706*
Euro OTC	Metoxisaleno	1608019	22785	40	20160913*
Euro OTC	Metoxisaleno	2106002	25702	50	20210623*
Fagron	Metoxisaleno	15J15-B03-321321	23165	40	20151124
Fagron	Metoxisaleno	18A12-B50-355102	24697	40	20181112

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 9 reference samples from the substance/substance group *Metoxisaleno*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.
- 152 552 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 480 spectra of 15 reference samples from the substance/substance group *Metoxisaleno*.
- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metoxisaleno	16103014	23166	40
Caelo	Metoxisaleno	191960	24760	40
Caelo	Metoxisaleno	22000545003	26312	30
Caelo	Metoxisaleno	24001655	27312	30
Euro OTC	Metoxisaleno	1802021	24070	40
Euro OTC	Metoxisaleno	1904009	24774	40
Euro OTC	Metoxisaleno	2006025	25319	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Metoxisaleno	2002046	25353	40
Euro OTC	Metoxisaleno	2211015	26528	40
Euro OTC	Metoxisaleno	2406012	27397	40
Fagron	Metoxisaleno	22D19-B01-218575	26291	30
Caelo	Metoxisaleno	22000545003	26312SI	20
Euro OTC	Metoxisaleno	2106002	25702SI[†]	10
Euro OTC	Metoxisaleno	2211015	26528SI	20
Fagron	Metoxisaleno	22D19-B01-218575	26291SI	20

- 201 604 spectra from a total of 4033 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 388 spectra from 205 *Apo-Ident* customers from 111 batches from the substance/substance group *Metoxisaleno*.

- Among them are spectra of independent samples from 106 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Metoxisaleno	2106002-01	2
	Metoxisaleno	22003782004	1
	Metoxisaleno	2211015-01	3
AHD	Metoxisaleno	15244204	1
AHD	Metoxisaleno	1608019-02	1
AHD	Metoxisaleno	16103019	1
AHD	Metoxisaleno	17078101	1
AHD	Metoxisaleno	17078108	2
Anzag	Metoxisaleno	1306041-01	1
Anzag	Metoxisaleno	2211015-01	1
Anzag	Metoxisaleno	APHCFMPC16011M	1
Apo-ident/Alliance	Metoxisaleno	1802021-01	1
Audor Pharma	Metoxisaleno	1203009M	1
Audor Pharma	Metoxisaleno	15244213	1
Audor Pharma	Metoxisaleno	AP1011024-01M	1
Audor Pharma	Metoxisaleno	AP15244213M	6
Audor Pharma	Metoxisaleno	APHCFMPC16011M	6
Audor Pharma	Metoxisaleno	APHCFMPC18003M	3
Bombastus	Metoxisaleno	15J15-B03-336704	1
Caelo	Metoxisaleno	1136428	1
Caelo	Metoxisaleno	11376413	2
Caelo	Metoxisaleno	11376420	1
Caelo	Metoxisaleno	11376433	1
Caelo	Metoxisaleno	1409003-01	5
Caelo	Metoxisaleno	1409003-02	1
Caelo	Metoxisaleno	14F06-B05-296501	1
Caelo	Metoxisaleno	1503009-01	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metoxisaleno	150613-01	1
Caelo	Metoxisaleno	15099802	1
Caelo	Metoxisaleno	15244204	3
Caelo	Metoxisaleno	15244205	2
Caelo	Metoxisaleno	15244209	1
Caelo	Metoxisaleno	15244211	1
Caelo	Metoxisaleno	15244216	1
Caelo	Metoxisaleno	16/079/M	1
Caelo	Metoxisaleno	1608019-02	2
Caelo	Metoxisaleno	16103004	1
Caelo	Metoxisaleno	16103008	1
Caelo	Metoxisaleno	17078101	2
Caelo	Metoxisaleno	17078107	1
Caelo	Metoxisaleno	17078108	3
Caelo	Metoxisaleno	17078114	2
Caelo	Metoxisaleno	1802021-01	3
Caelo	Metoxisaleno	18A12-B50-354863	1
Caelo	Metoxisaleno	190441001	1
Caelo	Metoxisaleno	190441002	3
Caelo	Metoxisaleno	19044103	5
Caelo	Metoxisaleno	19044107	2
Caelo	Metoxisaleno	190441074	1
Caelo	Metoxisaleno	19044108	1
Caelo	Metoxisaleno	19044110	7
Caelo	Metoxisaleno	1904411002	1
Caelo	Metoxisaleno	191960003	1
Caelo	Metoxisaleno	191960006	2
Caelo	Metoxisaleno	191960008	1
Caelo	Metoxisaleno	191960009	3
Caelo	Metoxisaleno	19196001	2
Caelo	Metoxisaleno	20002295002	3
Caelo	Metoxisaleno	20002295003	1
Caelo	Metoxisaleno	20002295004	1
Caelo	Metoxisaleno	20002295006	2
Caelo	Metoxisaleno	20002295010	1
Caelo	Metoxisaleno	20002295012	2
Caelo	Metoxisaleno	2002046-01	1
Caelo	Metoxisaleno	22000545001	1
Caelo	Metoxisaleno	22000545003	1
Caesar & Loretz GmbH...	Metoxisaleno	20002295003	1
Caesar & Loretz GmbH	Metoxisaleno	190441001	1
Caesar & Loretz GmbH	Metoxisaleno	19044103	2
Caesar & Loretz GmbH	Metoxisaleno	19044108	1
Caesar & Loretz GmbH	Metoxisaleno	19044110	2
Caesar & Loretz GmbH	Metoxisaleno	20002295003	1
Caesar & Loretz GmbH	Metoxisaleno	20002295007	2
Caesar&Lorenz	Metoxisaleno	20002295003	1
EU.RHO.Pharm	Metoxisaleno	2006025-02	2
EuRho/ AHD	Metoxisaleno	16103019	1
EuRho/ Phoenix	Metoxisaleno	2106002-01	2
EuRho/Fiebig	Metoxisaleno	1802021-01	1
EuRho/VDL	Metoxisaleno	1608019-02	1
EuRho	Metoxisaleno	1104010-01	1
EuRho	Metoxisaleno	2106002-01	2
Euro OCT	Metoxisaleno	1802021-01	1
Euro OCT	Metoxisaleno	1904009-01	1
Euro OCT	Metoxisaleno	1904009-02	1
Euro OTC	Metoxisaleno	1104010-01	1
Euro OTC	Metoxisaleno	1108019-01	1
Euro OTC	Metoxisaleno	1203009-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Metoxisaleno	120901501	1
Euro OTC	Metoxisaleno	1209015-01	4
Euro OTC	Metoxisaleno	130604101	1
Euro OTC	Metoxisaleno	1306041-01	5
Euro OTC	Metoxisaleno	1409003-01	5
Euro OTC	Metoxisaleno	140900302	1
Euro OTC	Metoxisaleno	1409003-02	3
Euro OTC	Metoxisaleno	150300901	1
Euro OTC	Metoxisaleno	1503009-01	12
Euro OTC	Metoxisaleno	1503009-02	9
Euro OTC	Metoxisaleno	1506013_01	1
Euro OTC	Metoxisaleno	1506013-01	19
Euro OTC	Metoxisaleno	1506013-02	7
Euro OTC	Metoxisaleno	1608019	1
Euro OTC	Metoxisaleno	1608019-01	4
Euro OTC	Metoxisaleno	160801902	1
Euro OTC	Metoxisaleno	1608019-02	18
Euro OTC	Metoxisaleno	1608019-1	1
Euro OTC	Metoxisaleno	1802021/01	1
Euro OTC	Metoxisaleno	1802021-01	40
Euro OTC	Metoxisaleno	1904009-01	25
Euro OTC	Metoxisaleno	1904009-02	1
Euro OTC	Metoxisaleno	2006025-01	4
Euro OTC	Metoxisaleno	2006025-02	1
Euro OTC	Metoxisaleno	2106002-01	13
Euro/Phönix	Metoxisaleno	1608019-02	1
Euroo	Metoxisaleno	1503009-01	1
Fag	Metoxisaleno	20f-12-F01	1
Fagron	Metoxisaleno	11D07-N16	1
Fagron	Metoxisaleno	11f21-n02	1
Fagron	Metoxisaleno	11F21-N02	1
Fagron	Metoxisaleno	12E02-N05	2
Fagron	Metoxisaleno	12G02-N14	1
Fagron	Metoxisaleno	14f06-b05-296500	1
Fagron	Metoxisaleno	14F06-B05-296500	1
Fagron	Metoxisaleno	14F06-B05-296501	2
Fagron	Metoxisaleno	14F06-B05-301978	1
Fagron	Metoxisaleno	150601301	1
Fagron	Metoxisaleno	15C10-B99-306266	1
Fagron	Metoxisaleno	15F23-B03	1
Fagron	Metoxisaleno	15F23-B03-309644	1
Fagron	Metoxisaleno	15F23-B03-316262	1
Fagron	Metoxisaleno	15F23-B03-318166	5
Fagron	Metoxisaleno	15J15-B03-321321	1
Fagron	Metoxisaleno	15J15-B03-341859	1
Fagron	Metoxisaleno	18A12-B50-359351	1
Fagron	Metoxisaleno	19H05-B02-366102	1
Fagron	Metoxisaleno	21111814	1
Fagron	Metoxisaleno	2111A-03262	2
Fagron	Metoxisaleno	B02-3661001	1
Fagron	Metoxisaleno	MS01/13-14	1
Franco / Ebert	Metoxisaleno	CMX-15/12	1
Herbal Creations/AHD	Metoxisaleno	APHCFMPC16011M	1
Herbal Creations/Cae…	Metoxisaleno	15244203	1
Herbal Creations/Cae…	Metoxisaleno	15244205	1
Herbal creations/Cae…	Metoxisaleno	15244208	1
Herbal creations/Cae…	Metoxisaleno	15244212	1
Herbal Creations	Metoxisaleno	1608019-01	1
L10	Metoxisaleno	2106002-01	2
Nachprüfung	Metoxisaleno	4211Q-03262	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Metoxisaleno	11D07-N16	2
Noweda	Metoxisaleno	140900302	1
Noweda	Metoxisaleno	19044103	2
Noweda	Metoxisaleno	2006025-01	1
Noweda	Metoxisaleno	2211015-01	1
PHOENIX 18.02.14	Metoxisaleno	1306041-01	2
Phoenix	Metoxisaleno	14F06-B05-296502	1
Phönix	Metoxisaleno	1608019-01	1
Phönix	Metoxisaleno	1608019-02	1
Phönix	Metoxisaleno	1802021-01	1
Phytoceut.Ltd	Metoxisaleno	1503009-01	3
Sanacorp	Metoxisaleno	1AKD6	1
Say Phytoceut. Ltd	Metoxisaleno	1209015-01	3

- 235 679 spectra from 1515 *Apo-Ident* customers from a total of 49 147 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metoxisaleno* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metoxisaleno* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	480	0	201 604
Type C	0	387	1	235 679

The substance/substance group *Metoxisaleno* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7500 %)
Type C	100.0000 % (> 99.9007 %)	99.7423 % (> 98.9691 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21555	21862	6,83	221,52
21862	21862	0,00	238,08
22785	22785	0,00	234,59
23165	21862	10,68	217,89
23167	21862	12,21	213,72
23333	23333	0,00	214,05
23346	23346	0,00	209,04
24697	21862	10,54	218,18
25702	25702	0,00	205,99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metronidazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20001-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metronidazol; Metronidazolum

Special notes

When selecting the *Metronidazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metronidazol	9	26	737

Second-stage model

For differentiation of the substance/substance group *Metronidazol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metronidazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	94,13	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metronidazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metronidazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metronidazol	12110410	20857	40	20120515
Caelo	Metronidazol	13095007	21356	40	20130426
Caelo	Metronidazol	13095007	21360	40	20130426
Caelo	Metronidazol	160892	22472	60	20160413*
Caelo	Metronidazol	20002297	25565	40	20200902*
Euro OTC	Metronidazol	1212030-02	21213	40	20130627
Euro OTC	Metronidazol	1508004	21881	60	20150819*
Euro OTC	Metronidazol	2005029	25330	40	20200820*
Fagron	Metronidazol	13D10-N02	21212	40	20130516
Fagron	Metronidazol	16I19-B04-326155	22835	40	20161013

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Metronidazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 522 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1130 spectra of 31 reference samples from the substance/substance group *Metronidazol*.

- Among them are spectra of independent samples from 26 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metronidazol	13095005	21214	40
Caelo	Metronidazol	172905	23808	40
Caelo	Metronidazol	190102	24558	40
Caelo	Metronidazol	21002293	25851	50
Caelo	Metronidazol	22002266	26490	40
Caelo	Metronidazol	23003075	27109	40
Euro OTC	Metronidazol	1609028	22751	40
Euro OTC	Metronidazol	1612013	22917	40
Euro OTC	Metronidazol	1701039	23132	40
Euro OTC	Metronidazol	1707008	23542	30
Euro OTC	Metronidazol	1706022	23550	30
Euro OTC	Metronidazol	1802007	23946	40
Euro OTC	Metronidazol	1807039	24203	40
Euro OTC	Metronidazol	1901042	24449	40
Euro OTC	Metronidazol	1906012	24766	40
Euro OTC	Metronidazol	1908028	24864	40
Euro OTC	Metronidazol	2007002	25328	40
Euro OTC	Metronidazol	2103002	25677	50
Euro OTC	Metronidazol	2207001	26199	40
Euro OTC	Metronidazol	2206031	26204	40
Euro OTC	Metronidazol	2308004	26888	40
Euro OTC	Metronidazol	2308003	26889	40
Euro OTC	Metronidazol	2402031	27145	40
Euro OTC	Metronidazol	2404007	27297	40
Fagron	Metronidazol	17C10-B04-355868	24586	40
Fagron	Metronidazol	21G29-B02-213325	26179	40
Caelo	Metronidazol	21002293	25851SI	10
Caelo	Metronidazol	22002266	26490SI	20
Euro OTC	Metronidazol	2207001	26199SI	20

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Metronidazol	2206031	26204SI	20
Fagron	Metronidazol	21G29-B02-213325	26179SI	20

- 200 954 spectra from a total of 4019 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5455 spectra from 1292 *Apo-Ident* customers from 779 batches from the substance/substance group *Metronidazol*.
- Among them are spectra of independent samples from 733 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Metronidazol		1
	Metronidazol	15253007	2
	Metronidazol	2005029-01	1
	Metronidazol	2007002-02	4
	Metronidazol	21002293005	1
	Metronidazol	21002293011	2
	Metronidazol	21002293016	4
	Metronidazol	21002293020	22
	Metronidazol	2103002-01	1
	Metronidazol	2103002-03	1
	Metronidazol	2103002-1	1
	Metronidazol	21G29-B02-213325	1
	Metronidazol	21G29-B02-221739	2
	Metronidazol	22002266002	4
	Metronidazol	22002266003	3
	Metronidazol	22002266004	7
	Metronidazol	22002266005	1
	Metronidazol	22002266006	9
	Metronidazol	22002266007	6
	Metronidazol	22002266008	24
	Metronidazol	22002266009	6
	Metronidazol	22002266010	20
	Metronidazol	2200226608	1
	Metronidazol	2202266003	1
	Metronidazol	2206031-01	3
	Metronidazol	2206031-02	1
	Metronidazol	2207001-01	4
	Metronidazol	230800-01	1
	Metronidazol	2308003-01	5
	Metronidazol	2308004-01	3
	Metronidazol	2308004-02	1
	Metronidazol	24000389002	4
	Metronidazol	24000389003	2
	Metronidazol	24000389006	1
17270001	Metronidazol	17058026	1
A.H. 19.02.13 ek: 5,86EUR	Metronidazol	12G04-N15	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
ACM	Metronidazol		1
AEP	Metronidazol	22002266008	1
Aep	Metronidazol	2202266008	1
AHD 03.02.17	Metronidazol	16089212	1
AHD 13.10.17 E.k:6,56	Metronidazol	17058003	1
AHD	Metronidazol	13214025	1
AHD	Metronidazol	15253005	1
AHD	Metronidazol	15253033	1
AHD	Metronidazol	16I19-B04-329160	2
AHD	Metronidazol	17290518	1
AHD	Metronidazol	19000516007	1
AHD	Metronidazol	21002293005	1
AHD	Metronidazol	21002293006	1
AHD	Metronidazol	21002293019	1
AHD	Metronidazol	22002266003	1
AHD	Metronidazol	22002266004	1
AHD	Metronidazol	220022660058	1
AHD	Metronidazol	22002266008	3
ALH	Metronidazol	1609028-01	1
Alliance Health 20.0...	Metronidazol	1307042-01	2
Alliance Health 23.0...	Metronidazol	1212001-02	1
Alliance Healthcare	Metronidazol	12110415	1
Alliance Healthcare	Metronidazol	20004568008	1
Alliance	Metronidazol	12339502	1
Alliance	Metronidazol	22002266008	1
alliance	Metronidazol	2206031-01	1
Allianz Healthcare	Metronidazol	19g02-b04	1
Anzag 21.10.14 EK 2.85	Metronidazol	13095007	1
Anzag 15.12.17 3.41	Metronidazol	1705812	1
Anzag	Metronidazol	11373512	1
anzag	Metronidazol	14C14-B02-291276	2
Anzag	Metronidazol	1505024-01	1
Anzag	Metronidazol	15253022	1
Anzag	Metronidazol	20004568005	1
Anzag;14,21EUR;16.04.15	Metronidazol	13214012	1
api-ident	Metronidazol	16/19-B04	1
Apo Ident	Metronidazol	1807039-03	1
Apoident,Phönix, 09....	Metronidazol	1701039-01	1
Apo-ident	Metronidazol	108703902	1
apo-ident	Metronidazol	1807039-01	2
apo-ident	Metronidazol	1901042-01	2
Apotheke an der Born...	Metronidazol	16089223	1
Audor Pharma	Metronidazol	1908028-02	1
Audor Pharma	Metronidazol	2007002-01	1
Bombastus	Metronidazol	123Validierung	1
Bombastus	Metronidazol	13214018	1
Bombastus	Metronidazol	15253032	1
Bombastus	Metronidazol	16089220	1
Bombastus	Metronidazol	1609028-01	1
Bombastus	Metronidazol	17C10-B04-346280	1
Bombastus	Metronidazol	18026401	1
Caelo	Metronidazol		7
Caelo	Metronidazol	10112903	1
Caelo	Metronidazol	10112907	1
Caelo	Metronidazol	102311870	1
Caelo	Metronidazol	10368310	1
Caelo	Metronidazol	10368311	1
Caelo	Metronidazol	10368313	1
Caelo	Metronidazol	10368318	1
Caelo	Metronidazol	10368319	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	1061804	2
Caelo	Metronidazol	1112028-01	1
Caelo	Metronidazol	11319807	1
Caelo	Metronidazol	11319810	2
Caelo	Metronidazol	11319812	1
Caelo	Metronidazol	11319816	2
Caelo	Metronidazol	11319818	2
Caelo	Metronidazol	11319819	1
Caelo	Metronidazol	11319823	5
Caelo	Metronidazol	11319824	2
Caelo	Metronidazol	11319825	3
Caelo	Metronidazol	113214021	1
Caelo	Metronidazol	11F15-N07	1
Caelo	Metronidazol	11h11-n03	1
Caelo	Metronidazol	1201156	1
Caelo	Metronidazol	12081507	1
Caelo	Metronidazol	12091403	1
Caelo	Metronidazol	1210411	1
Caelo	Metronidazol	12110105	1
Caelo	Metronidazol	12110403	1
Caelo	Metronidazol	12110405	8
Caelo	Metronidazol	121104085	1
Caelo	Metronidazol	12110411	5
Caelo	Metronidazol	12110412	5
Caelo	Metronidazol	12110413	4
Caelo	Metronidazol	12110414	3
Caelo	Metronidazol	12110415	4
Caelo	Metronidazol	12110421	6
Caelo	Metronidazol	12110422	16
Caelo	Metronidazol	12110423	1
Caelo	Metronidazol	121203001	2
Caelo	Metronidazol	1212030-21	1
Caelo	Metronidazol	12339501	7
Caelo	Metronidazol	12339502	18
Caelo	Metronidazol	12339503	6
Caelo	Metronidazol	12339504	6
Caelo	Metronidazol	12339507	7
Caelo	Metronidazol	12339508	4
Caelo	Metronidazol	12339509	4
Caelo	Metronidazol	12339510	10
Caelo	Metronidazol	12339511	14
Caelo	Metronidazol	12339519	12
Caelo	Metronidazol	12339520	4
Caelo	Metronidazol	12339521	1
Caelo	Metronidazol	12339526	1
Caelo	Metronidazol	12359501	1
Caelo	Metronidazol	1239504	1
Caelo	Metronidazol	12L17-N11	3
Caelo	Metronidazol	13041503	1
Caelo	Metronidazol	1307002	1
Caelo	Metronidazol	1307002-02	1
Caelo	Metronidazol	1307042-01	1
Caelo	Metronidazol	13095001	10
Caelo	Metronidazol	13095002	8
Caelo	Metronidazol	13095003	11
Caelo	Metronidazol	13095004	12
Caelo	Metronidazol	13095005	4
Caelo	Metronidazol	13095006	7
Caelo	Metronidazol	13095007	5
Caelo	Metronidazol	13095011	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	13095012	13
Caelo	Metronidazol	13095013	13
Caelo	Metronidazol	13095017	3
Caelo	Metronidazol	13095018	6
Caelo	Metronidazol	13095019	7
Caelo	Metronidazol	13095020	5
Caelo	Metronidazol	1314013	1
Caelo	Metronidazol	13214001	13
Caelo	Metronidazol	13214002	17
Caelo	Metronidazol	132140022	1
Caelo	Metronidazol	13214003	11
Caelo	Metronidazol	13214009	7
Caelo	Metronidazol	13214010	5
Caelo	Metronidazol	13214011	2
Caelo	Metronidazol	13214012	3
Caelo	Metronidazol	13214013	1
Caelo	Metronidazol	13214014	10
Caelo	Metronidazol	13214015	8
Caelo	Metronidazol	13214016	3
Caelo	Metronidazol	13214017	3
Caelo	Metronidazol	13214018	4
Caelo	Metronidazol	13214019	9
Caelo	Metronidazol	13214021	1
Caelo	Metronidazol	13214024	4
Caelo	Metronidazol	13214025	6
Caelo	Metronidazol	13214029	9
Caelo	Metronidazol	1321409	1
Caelo	Metronidazol	13J21-N07	1
Caelo	Metronidazol	1407003-01	1
Caelo	Metronidazol	1407003-2	1
Caelo	Metronidazol	14111304	1
Caelo	Metronidazol	1412016-01	4
Caelo	Metronidazol	1412016-02	1
Caelo	Metronidazol	14b27-b31-291230	1
Caelo	Metronidazol	14B27-B31-291230	1
Caelo	Metronidazol	14B27-B31-291234	1
Caelo	Metronidazol	14c14-b01-295545	1
Caelo	Metronidazol	14C14-B02-291237	1
Caelo	Metronidazol	14C14-B02-291239	1
Caelo	Metronidazol	14C14-B02-291276	1
Caelo	Metronidazol	1505024-02	2
Caelo	Metronidazol	1508004-01	2
Caelo	Metronidazol	1508004-02	1
Caelo	Metronidazol	15121202	1
Caelo	Metronidazol	15215103	4
Caelo	Metronidazol	15215104	5
Caelo	Metronidazol	15215105	1
Caelo	Metronidazol	15215106	5
Caelo	Metronidazol	15215107	1
Caelo	Metronidazol	15215108	10
Caelo	Metronidazol	1523006	1
Caelo	Metronidazol	1523013	1
Caelo	Metronidazol	1523017	1
Caelo	Metronidazol	1523026	1
Caelo	Metronidazol	1525016	1
Caelo	Metronidazol	15253001	13
Caelo	Metronidazol	15253002	5
Caelo	Metronidazol	15253003	9
Caelo	Metronidazol	15253004	14
Caelo	Metronidazol	15253005	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	15253006	10
Caelo	Metronidazol	15253007	13
Caelo	Metronidazol	15253011	11
Caelo	Metronidazol	15253013	12
Caelo	Metronidazol	15253013/2016030911	1
Caelo	Metronidazol	15253015	15
Caelo	Metronidazol	15253016	13
Caelo	Metronidazol	15253017	14
Caelo	Metronidazol	15253018	6
Caelo	Metronidazol	15253019	3
Caelo	Metronidazol	15253020	5
Caelo	Metronidazol	15253021	9
Caelo	Metronidazol	15253022	7
Caelo	Metronidazol	15253024	12
Caelo	Metronidazol	15253026	19
Caelo	Metronidazol	15253027	13
Caelo	Metronidazol	15253028	9
Caelo	Metronidazol	15253029	5
Caelo	Metronidazol	15253032	13
Caelo	Metronidazol	15253033	7
Caelo	Metronidazol	15253034	1
Caelo	Metronidazol	15258016	1
Caelo	Metronidazol	15A20-B07-303293	1
Caelo	Metronidazol	15A20-B07-303297	1
Caelo	Metronidazol	15A20-B07-303298	1
Caelo	Metronidazol	16/19-B04-326150	1
Caelo	Metronidazol	16/19-B04-326155	1
Caelo	Metronidazol	16/19-B04-329160	1
Caelo	Metronidazol	16051703	1
Caelo	Metronidazol	16056235	1
Caelo	Metronidazol	16089123	1
Caelo	Metronidazol	1608918	1
Caelo	Metronidazol	16089201	7
Caelo	Metronidazol	16089202	11
Caelo	Metronidazol	16089209	16
Caelo	Metronidazol	16089212	19
Caelo	Metronidazol	16089213	21
Caelo	Metronidazol	16089215	14
Caelo	Metronidazol	16089215/1140217	1
Caelo	Metronidazol	16089216	8
Caelo	Metronidazol	16089217	9
Caelo	Metronidazol	16089218	13
Caelo	Metronidazol	16089219	17
Caelo	Metronidazol	16089220	19
Caelo	Metronidazol	16089221	12
Caelo	Metronidazol	16089222	11
Caelo	Metronidazol	16089223	5
Caelo	Metronidazol	16089224	5
Caelo	Metronidazol	16089225	1
Caelo	Metronidazol	16089228	14
Caelo	Metronidazol	16089228-20170818Ma4	1
Caelo	Metronidazol	16089229	13
Caelo	Metronidazol	16089231	4
Caelo	Metronidazol	16089235	11
Caelo	Metronidazol	16089236	3
Caelo	Metronidazol	160892365302	1
Caelo	Metronidazol	160902801	1
Caelo	Metronidazol	1609028-01	7
Caelo	Metronidazol	161201301	1
Caelo	Metronidazol	1612013-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	1619-b04-326150	1
Caelo	Metronidazol	16253015	1
Caelo	Metronidazol	16D15-B50-324137	1
Caelo	Metronidazol	16I19-B04-329167	1
Caelo	Metronidazol	1701039-01	4
Caelo	Metronidazol	170580001	2
Caelo	Metronidazol	17058001	14
Caelo	Metronidazol	17058002	11
Caelo	Metronidazol	17058003	14
Caelo	Metronidazol	170580035444	1
Caelo	Metronidazol	17058004	9
Caelo	Metronidazol	17058005	14
Caelo	Metronidazol	1705801	1
Caelo	Metronidazol	17058010	14
Caelo	Metronidazol	17058011	18
Caelo	Metronidazol	17058012	21
Caelo	Metronidazol	17058012/2231117	1
Caelo	Metronidazol	170580123	1
Caelo	Metronidazol	17058013	17
Caelo	Metronidazol	17058013-20180404Ma4	1
Caelo	Metronidazol	17058013-20180619Ma6	1
Caelo	Metronidazol	17058014	20
Caelo	Metronidazol	17058015	19
Caelo	Metronidazol	17058016	27
Caelo	Metronidazol	170580165554	1
Caelo	Metronidazol	17058017	16
Caelo	Metronidazol	17058018	24
Caelo	Metronidazol	17058019	22
Caelo	Metronidazol	17058026	19
Caelo	Metronidazol	17058027	15
Caelo	Metronidazol	1706022-01	2
Caelo	Metronidazol	17070008-01	1
Caelo	Metronidazol	1707008-01	6
Caelo	Metronidazol	1707008-02	1
Caelo	Metronidazol	17250517	1
Caelo	Metronidazol	1729027	1
Caelo	Metronidazol	17290503	25
Caelo	Metronidazol	17290504	24
Caelo	Metronidazol	17290506	27
Caelo	Metronidazol	17290507	26
Caelo	Metronidazol	17290509	10
Caelo	Metronidazol	17290512	30
Caelo	Metronidazol	172905125723	1
Caelo	Metronidazol	17290513	5
Caelo	Metronidazol	17290515	3
Caelo	Metronidazol	17290517	51
Caelo	Metronidazol	17290518	58
Caelo	Metronidazol	17290519	10
Caelo	Metronidazol	17290525	52
Caelo	Metronidazol	17290526	15
Caelo	Metronidazol	17290527	49
Caelo	Metronidazol	17290532	34
Caelo	Metronidazol	17290533	31
Caelo	Metronidazol	17290534	3
Caelo	Metronidazol	17290625	1
Caelo	Metronidazol	172990507	1
Caelo	Metronidazol	174058019	1
Caelo	Metronidazol	175058013	1
Caelo	Metronidazol	1758017	1
Caelo	Metronidazol	1790504	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	1790512	1
Caelo	Metronidazol	1790517	1
Caelo	Metronidazol	179290525	1
Caelo	Metronidazol	17C10-B04-346275	2
Caelo	Metronidazol	17C10-B04-346280	1
Caelo	Metronidazol	1802007-01	1
Caelo	Metronidazol	180264001	1
Caelo	Metronidazol	18026401	14
Caelo	Metronidazol	18051201	1
Caelo	Metronidazol	18061803	1
Caelo	Metronidazol	1807039-01	2
Caelo	Metronidazol	1807039-03	1
Caelo	Metronidazol	18071401	1
Caelo	Metronidazol	18B28-B50	1
Caelo	Metronidazol	190000516008	1
Caelo	Metronidazol	1900016019	1
Caelo	Metronidazol	19000512012	1
Caelo	Metronidazol	190005160	1
Caelo	Metronidazol	19000516001	16
Caelo	Metronidazol	190005160016	1
Caelo	Metronidazol	19000516002	44
Caelo	Metronidazol	19000516003	8
Caelo	Metronidazol	19000516006	35
Caelo	Metronidazol	19000516007	34
Caelo	Metronidazol	19000516008	27
Caelo	Metronidazol	19000516010	40
Caelo	Metronidazol	190005-16010	1
Caelo	Metronidazol	19000516012	12
Caelo	Metronidazol	19000516016	33
Caelo	Metronidazol	19000516017	18
Caelo	Metronidazol	19000516019	19
Caelo	Metronidazol	1900214	1
Caelo	Metronidazol	1900516010	2
Caelo	Metronidazol	1901020	1
Caelo	Metronidazol	190102003	4
Caelo	Metronidazol	19010201	25
Caelo	Metronidazol	19010202	25
Caelo	Metronidazol	19010203	35
Caelo	Metronidazol	19010210	23
Caelo	Metronidazol	19010211	35
Caelo	Metronidazol	19010212	37
Caelo	Metronidazol	19010213	23
Caelo	Metronidazol	19010214	19
Caelo	Metronidazol	19010215	24
Caelo	Metronidazol	19010216	20
Caelo	Metronidazol	19011909	1
Caelo	Metronidazol	19012011	1
Caelo	Metronidazol	1901210	1
Caelo	Metronidazol	1901214	1
Caelo	Metronidazol	190601201	1
Caelo	Metronidazol	190802802	1
Caelo	Metronidazol	1910203	1
Caelo	Metronidazol	1957059	1
Caelo	Metronidazol	1957069	1
Caelo	Metronidazol	19G02-B04-362815	1
Caelo	Metronidazol	200004568003	1
Caelo	Metronidazol	200004568004	1
Caelo	Metronidazol	200004568005	1
Caelo	Metronidazol	200004568008	1
Caelo	Metronidazol	20001568016	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	20004567001	8
Caelo	Metronidazol	20004568001	2
Caelo	Metronidazol	200045680013	1
Caelo	Metronidazol	200045680016	1
Caelo	Metronidazol	20004568003	46
Caelo	Metronidazol	20004568004	30
Caelo	Metronidazol	20004568005	39
Caelo	Metronidazol	20004568008	9
Caelo	Metronidazol	20004568009	50
Caelo	Metronidazol	20004568012	2
Caelo	Metronidazol	20004568013	19
Caelo	Metronidazol	20004568015	18
Caelo	Metronidazol	20004568016	15
Caelo	Metronidazol	2000456809	1
Caelo	Metronidazol	2004568009	1
Caelo	Metronidazol	2004568016	1
Caelo	Metronidazol	200700201	1
Caelo	Metronidazol	200702-01	1
Caelo	Metronidazol	20121121	1
Caelo	Metronidazol	2013U-01870	1
Caelo	Metronidazol	20140612-12	1
Caelo	Metronidazol	2022015B	1
Caelo	Metronidazol	2071304	1
Caelo	Metronidazol	20G07f03372286	1
Caelo	Metronidazol	210002293014	1
Caelo	Metronidazol	210004568015	1
Caelo	Metronidazol	21002293002	5
Caelo	Metronidazol	21002293003	21
Caelo	Metronidazol	21002293004	6
Caelo	Metronidazol	21002293005	15
Caelo	Metronidazol	21002293006	22
Caelo	Metronidazol	21002293007	1
Caelo	Metronidazol	21002293009	10
Caelo	Metronidazol	21002293010	7
Caelo	Metronidazol	21002293011	12
Caelo	Metronidazol	21002293014	14
Caelo	Metronidazol	21002293016	9
Caelo	Metronidazol	21002293017	5
Caelo	Metronidazol	21002293019	3
Caelo	Metronidazol	21002293020	1
Caelo	Metronidazol	2100293005	1
Caelo	Metronidazol	220022656003	1
Caelo	Metronidazol	22002266003	5
Caelo	Metronidazol	22002266004	1
Caelo	Metronidazol	22002266006	5
Caelo	Metronidazol	2200226608	1
Caelo	Metronidazol	2202266003	1
Caelo	Metronidazol	220226606	1
Caelo	Metronidazol	22040734	1
Caelo	Metronidazol	23011504	1
Caelo	Metronidazol	23021713	1
Caelo	Metronidazol	2619A-01870	1
Caelo	Metronidazol	27092014A	1
Caelo	Metronidazol	2750	1
Caelo	Metronidazol	280218010	1
Caelo	Metronidazol	28061204	1
Caelo	Metronidazol	2813E1870	1
Caelo	Metronidazol	3112M-01870	1
Caelo	Metronidazol	320F01870	1
Caelo	Metronidazol	3301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazol	338(intern)	1
Caelo	Metronidazol	39/AKD16	1
Caelo	Metronidazol	39/AKD4	1
Caelo	Metronidazol	3947/V04/16	1
Caelo	Metronidazol	473800045689	1
Caelo	Metronidazol	49(17290526)	1
Caelo	Metronidazol	51(19000516012)	1
Caelo	Metronidazol	6003	1
Caelo	Metronidazol	604081626	1
Caelo	Metronidazol	607211870	1
Caelo	Metronidazol	614U1870	1
Caelo	Metronidazol	7031401	1
Caelo	Metronidazol	7071405	1
Caelo	Metronidazol	7091714	1
Caelo	Metronidazol	8012014B	1
Caelo	Metronidazol	820I-01870	1
Caelo	Metronidazol	9715621	1
Caelo	Metronidazol	C04171127	1
Caelo	Metronidazol	ch17290513	1
Caelo	Metronidazol	F170013	1
Caelo	Metronidazol	I-13095005	1
Caelo	Metronidazol	MZ3847368	1
Caeolo/Phönix	Metronidazol	16089228	1
Caeolo/Sanacorp	Metronidazol	17058019	1
Caeolo/Sanacorp	Metronidazol	17290518	1
Caesar & Lorenz GmbH	Metronidazol	15253013	1
Caesar & Lorenz/Hold...	Metronidazol	20004568013	2
Caesar & Lorenz	Metronidazol	13095013	1
Caesar & Loretz / AHD	Metronidazol	19000516008	1
Caesar & Loretz / AHD	Metronidazol	19010210	2
Caesar & Loretz /Phönix	Metronidazol	19000516007	1
Caesar & Loretz GmbH...	Metronidazol	17058001	1
Caesar & Loretz GmbH...	Metronidazol	17290532	1
Caesar & Loretz GmbH...	Metronidazol	19000516007	1
Caesar & Loretz GmbH...	Metronidazol	19000516017	1
Caesar & Loretz GmbH...	Metronidazol	19010215	1
Caesar & Loretz GmbH...	Metronidazol	20004568009	1
Caesar & Loretz GmbH...	Metronidazol	20004568016	2
Caesar & Loretz GmbH...	Metronidazol	21002293019	1
Caesar & Loretz GmbH...	Metronidazol	22002266003	1
Caesar & Loretz GmbH...	Metronidazol	19000516006	1
Caesar & Loretz GmbH...	Metronidazol	20004568016	1
Caesar & Loretz GmbH...	Metronidazol	19010212	1
Caesar & Loretz GmbH...	Metronidazol	19010213	1
Caesar & Loretz GmbH...	Metronidazol	19000516016	1
Caesar & Loretz GmbH...	Metronidazol	21002293010	1
Caesar & Loretz GmbH...	Metronidazol	19010214	1
Caesar & Loretz GmbH...	Metronidazol	19000516016	1
Caesar & Loretz GmbH...	Metronidazol	21002293003	1
Caesar & Loretz GmbH...	Metronidazol	19000516006	1
Caesar & Loretz GmbH...	Metronidazol	19010211	1
Caesar & Loretz GmbH...	Metronidazol	19000516002	1
Caesar & Loretz GmbH...	Metronidazol	19000516019	1
Caesar & Loretz GmbH...	Metronidazol	19010214	1
Caesar & Loretz GmbH...	Metronidazol	21002293006	1
Caesar & Loretz GmbH...	Metronidazol	17290525	1
Caesar & Loretz GmbH...	Metronidazol	21002293006	1
Caesar & Loretz GmbH...	Metronidazol	21002293010	1
Caesar & Loretz GmbH...	Metronidazol	19000516002	1
Caesar & Loretz GmbH...	Metronidazol	19010203	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Metronidazol	20004568003	1
Caesar & Loretz GmbH/AHD	Metronidazol	19000516006	1
Caesar & Loretz GmbH/AHD	Metronidazol	20004568013	1
Caesar & Loretz GmbH/AHD	Metronidazol	21002293002	1
Caesar & Loretz GmbH/AHD	Metronidazol	21002293011	1
Caesar & Loretz GmbH...	Metronidazol	20004568004	2
Caesar & Loretz GmbH...	Metronidazol	19000516002	1
Caesar & Loretz GmbH...	Metronidazol	19000516019	1
Caesar & Loretz GmbH...	Metronidazol	20004568009	1
Caesar & Loretz GmbH...	Metronidazol	21002293009	1
Caesar & Loretz GmbH/G	Metronidazol	19010211	1
Caesar & Loretz GmbH/G	Metronidazol	20004568009	1
Caesar & Loretz GmbH/Gehe	Metronidazol	19000516001	1
Caesar & Loretz GmbH/Gehe	Metronidazol	19000516007	1
Caesar & Loretz GmbH/gehe	Metronidazol	19000516008	2
Caesar & Loretz GmbH/Gehe	Metronidazol	19010201	2
Caesar & Loretz GmbH/gehe	Metronidazol	19010202	1
Caesar & Loretz GmbH/Gehe	Metronidazol	1908028-01	1
Caesar & Loretz GmbH/Gehe	Metronidazol	20004568005	1
Caesar & Loretz GmbH/GEHE	Metronidazol	20004568016	1
Caesar & Loretz GmbH/Gehe	Metronidazol	21002293005	1
Caesar & Loretz GmbH...	Metronidazol	19000516003	1
Caesar & Loretz GmbH...	Metronidazol	21002293010	2
Caesar & Loretz GmbH...	Metronidazol	19010214	1
Caesar & Loretz GmbH...	Metronidazol	21002293003	1
Caesar & Loretz GmbH...	Metronidazol	19000516002	1
Caesar & Loretz GmbH...	Metronidazol	20004568003	2
Caesar & Loretz GmbH...	Metronidazol	21002293003	3
Caesar & Loretz GmbH...	Metronidazol	1807039-02	1
Caesar & Loretz GmbH...	Metronidazol	190102003	1
Caesar & Loretz GmbH...	Metronidazol	19010212	1
Caesar & Loretz GmbH...	Metronidazol	19010213	1
Caesar & Loretz GmbH...	Metronidazol	20004567001	1
Caesar & Loretz GmbH...	Metronidazol	20004568005	1
Caesar & Loretz GmbH...	Metronidazol	21002293004	1
Caesar & Loretz GmbH/K	Metronidazol	20004568005	1
Caesar & Loretz GmbH/Kehr	Metronidazol	19000516016	1
Caesar & Loretz GmbH...	Metronidazol	19000516007	1
Caesar & Loretz GmbH...	Metronidazol	20004568003	1
Caesar & Loretz GmbH...	Metronidazol	20004568005	1
Caesar & Loretz GmbH...	Metronidazol	19000516002	1
Caesar & Loretz GmbH...	Metronidazol	19000516010	5
Caesar & Loretz GmbH...	Metronidazol	19010203	2
Caesar & Loretz GmbH...	Metronidazol	21002293009	1
Caesar & Loretz GmbH/Ph	Metronidazol	19010212	2
Caesar & Loretz GmbH/PHoe	Metronidazol	19000516010	1
Caesar & Loretz GmbH...	Metronidazol	19000516007	1
Caesar & Loretz GmbH...	Metronidazol	19010210	1
Caesar & Loretz GmbH...	Metronidazol	17290527	1
Caesar & Loretz GmbH...	Metronidazol	19010215	1
Caesar & Loretz GmbH...	Metronidazol	20004568003	1
Caesar & Loretz GmbH...	Metronidazol	20004568009	1
Caesar & Loretz GmbH...	Metronidazol	20004568013	2
Caesar & Loretz GmbH...	Metronidazol	20004568016	1
Caesar & Loretz GmbH...	Metronidazol	22002266008	1
Caesar & Loretz GmbH...	Metronidazol	19000516010	1
Caesar & Loretz GmbH...	Metronidazol	19000516012	1
Caesar & Loretz GmbH...	Metronidazol	19000516017	2
Caesar & Loretz GmbH...	Metronidazol	19010213	2
Caesar & Loretz GmbH...	Metronidazol	20004568004	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Metronidazol	20004568009	2
Caesar & Loretz GmbH...	Metronidazol	21002293004	1
Caesar & Loretz GmbH...	Metronidazol	21002293009	1
Caesar & Loretz GmbH...	Metronidazol	21002293010	1
Caesar & Loretz GmbH...	Metronidazol	22002266003	1
Caesar & Loretz GmbH...	Metronidazol	AP220630-01	1
Caesar & Loretz GmbH	Metronidazol	15253017	1
Caesar & Loretz GmbH	Metronidazol	16089224	1
Caesar & Loretz GmbH	Metronidazol	17058027	1
Caesar & Loretz GmbH	Metronidazol	17290504	3
Caesar & Loretz GmbH	Metronidazol	17290512	1
Caesar & Loretz GmbH	Metronidazol	17290517	6
Caesar & Loretz GmbH	Metronidazol	17290518	2
Caesar & Loretz GmbH	Metronidazol	17290525	10
Caesar & Loretz GmbH	Metronidazol	17290526	7
Caesar & Loretz GmbH	Metronidazol	17290527	7
Caesar & Loretz GmbH	Metronidazol	17290532	2
Caesar & Loretz GmbH	Metronidazol	17290533	4
Caesar & Loretz GmbH	Metronidazol	17290534	2
Caesar & Loretz GmbH	Metronidazol	19000516001	4
Caesar & Loretz GmbH	Metronidazol	19000516002	12
Caesar & Loretz GmbH	Metronidazol	19000516006	11
Caesar & Loretz GmbH	Metronidazol	19000516007	8
Caesar & Loretz GmbH	Metronidazol	19000516008	13
Caesar & Loretz GmbH	Metronidazol	19000516010	14
Caesar & Loretz GmbH	Metronidazol	19000516012	11
Caesar & Loretz GmbH	Metronidazol	19000516016	9
Caesar & Loretz GmbH	Metronidazol	19000516017	10
Caesar & Loretz GmbH	Metronidazol	19000516019	4
Caesar & Loretz GmbH	Metronidazol	190102002	1
Caesar & Loretz GmbH	Metronidazol	190102003	2
Caesar & Loretz GmbH	Metronidazol	19010201	4
Caesar & Loretz GmbH	Metronidazol	19010202	10
Caesar & Loretz GmbH	Metronidazol	19010203	12
Caesar & Loretz GmbH	Metronidazol	19010210	5
Caesar & Loretz GmbH	Metronidazol	19010211	15
Caesar & Loretz GmbH	Metronidazol	19010212	6
Caesar & Loretz GmbH	Metronidazol	19010213	8
Caesar & Loretz GmbH	Metronidazol	19010214	4
Caesar & Loretz GmbH	Metronidazol	19010215	1
Caesar & Loretz GmbH	Metronidazol	19010216	5
Caesar & Loretz GmbH	Metronidazol	19G02	1
Caesar & Loretz GmbH	Metronidazol	19G02-B04	1
Caesar & Loretz GmbH	Metronidazol	20004567001	2
Caesar & Loretz GmbH	Metronidazol	20004568003	13
Caesar & Loretz GmbH	Metronidazol	20004568004	19
Caesar & Loretz GmbH	Metronidazol	20004568005	25
Caesar & Loretz GmbH	Metronidazol	20004568008	7
Caesar & Loretz GmbH	Metronidazol	20004568009	17
Caesar & Loretz GmbH	Metronidazol	20004568013	5
Caesar & Loretz GmbH	Metronidazol	20004568015	1
Caesar & Loretz GmbH	Metronidazol	20004568016	13
Caesar & Loretz GmbH	Metronidazol	21002293002	2
Caesar & Loretz GmbH	Metronidazol	21002293003	6
Caesar & Loretz GmbH	Metronidazol	21002293004	6
Caesar & Loretz GmbH	Metronidazol	21002293005	7
Caesar & Loretz GmbH	Metronidazol	21002293006	8
Caesar & Loretz GmbH	Metronidazol	21002293007	1
Caesar & Loretz GmbH	Metronidazol	21002293009	2
Caesar & Loretz GmbH	Metronidazol	21002293010	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Metronidazol	21002293011	4
Caesar & Loretz GmbH	Metronidazol	21002293014	7
Caesar & Loretz GmbH	Metronidazol	21002293017	7
Caesar & Loretz GmbH	Metronidazol	21002293019	3
Caesar & Loretz GmbH	Metronidazol	21002293020	1
Caesar & Loretz GmbH	Metronidazol	22002266003	3
Caesar & Loretz GmbH	Metronidazol	22002266006	2
Caesar & Loretz GmbH	Metronidazol	22002266007	2
Caesar & Loretz GmbH	Metronidazol	22002266008	1
Caesar & Loretz GmbH	Metronidazol	9000516006	1
Caesar & Loretz GmbH...	Metronidazol	19010202	1
Caesar & Loretz GmbH...	Metronidazol	19G02-B04-362816	1
Caesar & Loretz Hilden	Metronidazol	17290518	1
Caesar & Loretz Hilden	Metronidazol	19000516008	1
Caesar & Loretz Hilden	Metronidazol	19010212	1
Caesar & Loretz Hilden	Metronidazol	19010214	1
Caesar & Loretz/AHD	Metronidazol	19000516010	1
Caesar & Loretz/Geil...	Metronidazol	17290525	1
Caesar & Loretz/Geil...	Metronidazol	19000516008	1
Caesar & Loretz/Geil...	Metronidazol	19010211	1
Caesar & Loretz/Noweda	Metronidazol	20004568009	1
Caesar & Loretz	Metronidazol	16089212	1
Caesar & Loretz	Metronidazol	17058003	1
Caesar & Loretz	Metronidazol	17058019	1
Caesar & Loretz	Metronidazol	17290512	1
Caesar Loretz	Metronidazol	19000516006	1
Caesar u. Loretz GmbH	Metronidazol	19000516008	1
Caesar u. Loretz GmbH	Metronidazol	19000516016	1
Caesar u. Loretz GmbH	Metronidazol	20004568009	1
Caesar und Loretz GmbH	Metronidazol	17290503	1
Caesar&Lorenz/AHD	Metronidazol	17290506	1
Caesar&Lorenz	Metronidazol	20004568003	2
Caesar&Lorenz	Metronidazol	21002293002	3
Caesar&Lorenz	Metronidazol	21002293003	1
Caesar&Loretz GmbH/Anzag	Metronidazol	12339511	1
Caesar&Loretz GmbH/S...	Metronidazol	15253003	1
Caesar&Loretz GmbH	Metronidazol	19000516019	1
Caesar&Loretz GmbH	Metronidazol	19010210	1
Caesar&Loretz GmbH	Metronidazol	21002293009	1
Caesar&loretz,Phoenix	Metronidazol	12110410	1
Cealo/ Gehe	Metronidazol	19010213	1
Cealo/Gehe	Metronidazol	17290506	1
cealo/Gehe	Metronidazol	20004568003	1
Cealo/Phoenix	Metronidazol	21002293011	1
Cealo/Sanacorp	Metronidazol	13095003	1
Cealo/Sanacorp	Metronidazol	1900051610	1
Cealo	Metronidazol	16089219	1
Cealo	Metronidazol	19000516001	1
Cealo	Metronidazol	20004568015	1
celo / Gehe	Metronidazol	123456	1
celo	Metronidazol	20004568003	3
Corden Pharma / Gehe	Metronidazol	17290504	1
Corden Pharma Bergam...	Metronidazol	C3356	1
Corden Pharma Bergamo S.p	Metronidazol	1807039-02	2
Corden Pharma Bergam...	Metronidazol	19010214	1
Corden Pharma Bergam...	Metronidazol	F180012	1
Corden Pharma	Metronidazol	1212001-02	2
Corden/ Gehe	Metronidazol	2207001-01	1
Corden/Noweda	Metronidazol	19010210	1
Corden/Noweda	Metronidazol	F180029	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Delta	Metronidazol	17058001	1
Delta	Metronidazol	17290503	2
E Plus	Metronidazol	1707008-01	1
Ebert & Jacobi	Metronidazol	1609028-01	2
Ebert	Metronidazol	1412016-02	1
Ebert-Jacobi	Metronidazol	16089224	1
Eu Rho	Metronidazol	2007002-02	1
EuRho / Noweda	Metronidazol	1807039-03	3
EuRho/AHD	Metronidazol	1906012-01	1
EuRho/Jenne	Metronidazol	1802007-02	1
EuRho/Noweda	Metronidazol	180601M1706022-01	1
EuRho/Noweda	Metronidazol	2007002-01	1
EuRho/Phoenix	Metronidazol	2007002-02	1
EuRho/Phönix	Metronidazol	1307002-01	1
EuRho	Metronidazol	110903002	1
EuRho	Metronidazol	1109030-02	1
EuRho	Metronidazol	1212001-02	1
EuRho	Metronidazol	1307042-02	1
Eurho	Metronidazol	1406010-01	1
EuRho	Metronidazol	1406010-01	1
EuRho	Metronidazol	1407003-01	1
EuRho	Metronidazol	1412016-01	1
eurho	Metronidazol	1612013-01	1
EuRho	Metronidazol	1612013-02	5
EuRho	Metronidazol	170103901	1
EuRho	Metronidazol	1701039-01	2
EuRho	Metronidazol	1706022-02	1
EuRho	Metronidazol	1707008-01	1
EuRho	Metronidazol	1802007-02	2
Eurho	Metronidazol	1807039-01	1
EuRho	Metronidazol	1807039-01	2
EuRho	Metronidazol	180703902	1
EuRho	Metronidazol	1807039-02	1
Eurho	Metronidazol	1908028-01	1
EuRho	Metronidazol	2005029-01	1
Eurimpharm	Metronidazol	140601001	1
EURO / Sanacorp	Metronidazol	160902801	1
Euro Gehe	Metronidazol	1707008-01	1
Euro OCT / Krieger	Metronidazol	1908028-02	1
Euro OTC	Metronidazol		4
Euro OTC	Metronidazol	10800401	1
Euro OTC	Metronidazol	1109016-01	1
Euro OTC	Metronidazol	1109030-01	7
Euro OTC	Metronidazol	110903002	1
Euro OTC	Metronidazol	1109030-02	1
Euro OTC	Metronidazol	1109030-03	2
Euro OTC	Metronidazol	1112028-01	4
Euro OTC	Metronidazol	1112028-02	7
Euro OTC	Metronidazol	121001-02	3
Euro OTC	Metronidazol	1212001-01	8
Euro OTC	Metronidazol	1212001-02	13
Euro OTC	Metronidazol	1212030-01	3
Euro OTC	Metronidazol	1212030-02	7
Euro OTC	Metronidazol	1220141155F	1
Euro OTC	Metronidazol	128061/72	1
Euro OTC	Metronidazol	13070002-02	1
Euro OTC	Metronidazol	1307002-01	11
Euro OTC	Metronidazol	1307002-02	1
Euro OTC	Metronidazol	130704201	1
Euro OTC	Metronidazol	1307042-01	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Metronidazol	1307042-02	7
Euro OTC	Metronidazol	1308704201	1
Euro OTC	Metronidazol	13214010	1
Euro OTC	Metronidazol	13B06-N03	1
Euro OTC	Metronidazol	140601001	2
Euro OTC	Metronidazol	1406010-01	21
Euro OTC	Metronidazol	1407003	1
Euro OTC	Metronidazol	140700301	1
Euro OTC	Metronidazol	1407003-01	7
Euro OTC	Metronidazol	140700302	2
Euro OTC	Metronidazol	1407003-02	10
Euro OTC	Metronidazol	1412016	1
Euro OTC	Metronidazol	1412016-01	15
Euro OTC	Metronidazol	1412016-02	26
Euro OTC	Metronidazol	14120601	1
Euro OTC	Metronidazol	1418E-01870	1
Euro OTC	Metronidazol	1503004-01	1
Euro OTC	Metronidazol	150502401	4
Euro OTC	Metronidazol	1505024-01	14
Euro OTC	Metronidazol	150502402	1
Euro OTC	Metronidazol	1505024-02	7
Euro OTC	Metronidazol	1505024-03	3
Euro OTC	Metronidazol	150800	1
Euro OTC	Metronidazol	1508004	1
Euro OTC	Metronidazol	150800401	1
Euro OTC	Metronidazol	1508004-01	27
Euro OTC	Metronidazol	1508004-02	13
Euro OTC	Metronidazol	150804-01	1
Euro OTC	Metronidazol	15a20-b07-303294	1
Euro OTC	Metronidazol	15A20-B07-308525	2
Euro OTC	Metronidazol	1606028	1
Euro OTC	Metronidazol	16089222	1
Euro OTC	Metronidazol	16089224	1
Euro OTC	Metronidazol	1609023-01	1
Euro OTC	Metronidazol	1609028	3
Euro OTC	Metronidazol	1609028-01	31
Euro OTC	Metronidazol	1609028-02	13
Euro OTC	Metronidazol	161201301	1
Euro OTC	Metronidazol	1612013-01	28
Euro OTC	Metronidazol	1612013-02	3
Euro OTC	Metronidazol	169028-01	1
Euro OTC	Metronidazol	1701039	2
Euro OTC	Metronidazol	170103901	1
Euro OTC	Metronidazol	1701039-01	55
Euro OTC	Metronidazol	170139-01	2
Euro OTC	Metronidazol	1703028-01	1
Euro OTC	Metronidazol	17058005	1
Euro OTC	Metronidazol	1706022_01	1
Euro OTC	Metronidazol	170602201	1
Euro OTC	Metronidazol	1706022-01	16
Euro OTC	Metronidazol	1706022-02	3
Euro OTC	Metronidazol	1707008-002	1
Euro OTC	Metronidazol	170700801	3
Euro OTC	Metronidazol	1707008-01	57
Euro OTC	Metronidazol	170700802	1
Euro OTC	Metronidazol	1707008-02	10
Euro OTC	Metronidazol	1707039-01	1
Euro OTC	Metronidazol	1707088-01	2
Euro OTC	Metronidazol	17290513	1
Euro OTC	Metronidazol	176022-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Metronidazol	180200701	1
Euro OTC	Metronidazol	1802007-01	14
Euro OTC	Metronidazol	1802007-02	4
Euro OTC	Metronidazol	1807030-01	1
Euro OTC	Metronidazol	1807031-01	1
Euro OTC	Metronidazol	1807039	2
Euro OTC	Metronidazol	1807039/01	1
Euro OTC	Metronidazol	1807039-01	40
Euro OTC	Metronidazol	180703902	1
Euro OTC	Metronidazol	1807039-02	33
Euro OTC	Metronidazol	1807039-03	20
Euro OTC	Metronidazol	19010210	1
Euro OTC	Metronidazol	190104201	3
Euro OTC	Metronidazol	1901042-01	14
Euro OTC	Metronidazol	190104202	1
Euro OTC	Metronidazol	1901042-02	11
Euro OTC	Metronidazol	190601201	1
Euro OTC	Metronidazol	1906012-01	29
Euro OTC	Metronidazol	1906012-02	23
Euro OTC	Metronidazol	1908028	3
Euro OTC	Metronidazol	190802801	1
Euro OTC	Metronidazol	1908028-01	10
Euro OTC	Metronidazol	190802802	1
Euro OTC	Metronidazol	1908028-02	16
Euro OTC	Metronidazol	1908028-1	1
Euro OTC	Metronidazol	20004568015	1
Euro OTC	Metronidazol	2005029-01	19
Euro OTC	Metronidazol	200502902	1
Euro OTC	Metronidazol	2005029-02	4
Euro OTC	Metronidazol	20070002-02	1
Euro OTC	Metronidazol	200700201	3
Euro OTC	Metronidazol	2007002-01	52
Euro OTC	Metronidazol	2007002-02	24
Euro OTC	Metronidazol	20111025	1
Euro OTC	Metronidazol	2103002-01	11
Euro OTC	Metronidazol	2103002-02	1
Euro OTC	Metronidazol	2103002-03	5
Euro OTC	Metronidazol	2206031-01	3
Euro OTC	Metronidazol	2207001_01	1
Euro OTC	Metronidazol	2207001-01	4
Euro OTC	Metronidazol	2308003-01	1
Euro OTC	Metronidazol	300915ME	1
Euro OTC	Metronidazol	4516E-01870	1
Euro OTC	Metronidazol	700837	1
Euro OTC	Metronidazol	C04-160812	1
Euro OTC	Metronidazol	C04-171127	1
Euro OTC	Metronidazol	F120017	1
Euro OTC	Metronidazol	F160028	1
Euro OTC	Metronidazol	F1800012	1
Euro OTC	Metronidazol	F190012	1
Euro OTC	Metronidazol	F200019	1
Euro/ Sanacorp	Metronidazol	150800402	1
Euro/Anzag	Metronidazol	1807039-02	1
Euro/Noweda	Metronidazol	1609028-01	1
Euro/Sanacorp	Metronidazol	1609028	1
EuroPharma	Metronidazol	141201601	1
EurRho/Noweda	Metronidazol	1908028-02	1
Fagro/Sanacorp	Metronidazol	18B28-B50	1
Fagro	Metronidazol	14C14-B01-295548	1
Fagron	Metronidazol		5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazol	10F23-N05	1
Fagron	Metronidazol	112356	1
Fagron	Metronidazol	11C21-N01	1
Fagron	Metronidazol	11F15-N07	1
Fagron	Metronidazol	11J07-N07	1
Fagron	Metronidazol	1220141155F	2
Fagron	Metronidazol	12A20-B07-303298	1
Fagron	Metronidazol	12a2o-n18	1
Fagron	Metronidazol	12D30-N02	1
Fagron	Metronidazol	12d30-n03	1
Fagron	Metronidazol	12D30-N03	4
Fagron	Metronidazol	12f15-n04	1
Fagron	Metronidazol	12F15-N04	7
Fagron	Metronidazol	12G04-N15	15
Fagron	Metronidazol	12L17_N16	1
Fagron	Metronidazol	12l17-n11	1
Fagron	Metronidazol	12l17-N11	1
Fagron	Metronidazol	12L17N11	1
Fagron	Metronidazol	12L17-N11	15
Fagron	Metronidazol	12L17-N16	6
Fagron	Metronidazol	12L-N11	1
Fagron	Metronidazol	13/10-No3	1
Fagron	Metronidazol	13/21-N07	1
Fagron	Metronidazol	13/21-N7	2
Fagron	Metronidazol	13095002	1
Fagron	Metronidazol	13B06N03	1
Fagron	Metronidazol	13B06-N03	10
Fagron	Metronidazol	13D08N22	1
Fagron	Metronidazol	13D08-N22	6
Fagron	Metronidazol	13D10-N02	4
Fagron	Metronidazol	13I10-N03	3
Fagron	Metronidazol	13j21-n07	2
Fagron	Metronidazol	13j21-N07	1
Fagron	Metronidazol	13J21N07	2
Fagron	Metronidazol	13J21-N07	35
Fagron	Metronidazol	140700301	1
Fagron	Metronidazol	1412016-01	1
Fagron	Metronidazol	1414-B02-291237	1
Fagron	Metronidazol	141C14-B02-296437	1
Fagron	Metronidazol	14B27-B31-291234	1
Fagron	Metronidazol	14B27-B31-291235	1
Fagron	Metronidazol	14C12-B02-300182	1
Fagron	Metronidazol	14C14-802-291237	1
Fagron	Metronidazol	14C14-B01	1
Fagron	Metronidazol	14c14-B01-295545	1
Fagron	Metronidazol	14C14-B01-295548	1
Fagron	Metronidazol	14C14-B01-306363	5
Fagron	Metronidazol	14C14-B01-309058	2
Fagron	Metronidazol	14C14B02	3
Fagron	Metronidazol	14C14-B02	4
Fagron	Metronidazol	14C14-B02_291238	1
Fagron	Metronidazol	14C14-B02-2911239	1
Fagron	Metronidazol	14C14-B02-291237	9
Fagron	Metronidazol	14C14-B02-291238	2
Fagron	Metronidazol	14c14-b02-291239	1
Fagron	Metronidazol	14C14-B02-291239	7
Fagron	Metronidazol	14C14-B02-291241	1
Fagron	Metronidazol	14c14-b02-291275	1
Fagron	Metronidazol	14C14-B02-291275	4
Fagron	Metronidazol	14c14b02291276	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazol	14c14-b02-291276	2
Fagron	Metronidazol	14C14B02-291276	2
Fagron	Metronidazol	14C14-B02-291276	3
Fagron	Metronidazol	14C14-B02-295603	1
Fagron	Metronidazol	14C14-B02-296437	10
Fagron	Metronidazol	14-C14-B02-296437	1
Fagron	Metronidazol	14C14-B02-300182	4
Fagron	Metronidazol	14C14-B291237	1
Fagron	Metronidazol	14C14-Bo2-291276	1
Fagron	Metronidazol	1508004-01	1
Fagron	Metronidazol	15253017	2
Fagron	Metronidazol	15A20/B07-303298	1
Fagron	Metronidazol	15A20-B07	1
Fagron	Metronidazol	15A20-B07-303293	9
Fagron	Metronidazol	15A20-B07-303294	3
Fagron	Metronidazol	15A20-B07-303294Mg	1
Fagron	Metronidazol	15A20-B07-303295	1
Fagron	Metronidazol	15a20b07303298	1
Fagron	Metronidazol	15A20-B07-303298	8
Fagron	Metronidazol	15a20-b07-308196	1
Fagron	Metronidazol	15A20-B07-308196	3
Fagron	Metronidazol	15A20-B07-308198	1
Fagron	Metronidazol	15A20B07308525	1
Fagron	Metronidazol	15A20-B07-308525	6
Fagron	Metronidazol	15a20-b07-308791	1
Fagron	Metronidazol	15A20-B07-308791	4
Fagron	Metronidazol	15A20-B07312057	1
Fagron	Metronidazol	15A20-B07-312057	4
Fagron	Metronidazol	15A20-B07-312225	3
Fagron	Metronidazol	15A20-B07-31225	1
Fagron	Metronidazol	15A20Bo7308196	1
Fagron	Metronidazol	16/16-B04-326151	1
Fagron	Metronidazol	16/19-B04	3
Fagron	Metronidazol	16/19-B04-326150	6
Fagron	Metronidazol	16/19-B04-326151	3
Fagron	Metronidazol	16/19-B04-326152	1
Fagron	Metronidazol	16/19-B04-326154	1
Fagron	Metronidazol	16/19-B04-326155	2
Fagron	Metronidazol	16/19-B04-329160	1
Fagron	Metronidazol	16/19-B04-329162	1
Fagron	Metronidazol	16/19-B04-329163	1
Fagron	Metronidazol	16/19-B04-329167	2
Fagron	Metronidazol	16/19-b04-329168	1
Fagron	Metronidazol	16/19-B04-329168	3
Fagron	Metronidazol	16/19bo4326155	1
Fagron	Metronidazol	160902	1
Fagron	Metronidazol	1609028-01	2
Fagron	Metronidazol	1612013-01	3
Fagron	Metronidazol	1619-B04-326150	1
Fagron	Metronidazol	1619b04326155	1
Fagron	Metronidazol	1619-B04-326155	1
Fagron	Metronidazol	1619B04329161	1
Fagron	Metronidazol	16D15-B50-324137	2
Fagron	Metronidazol	16H15-B50-326734	1
Fagron	Metronidazol	16I19-B04	5
Fagron	Metronidazol	16I19-B04-326150	3
Fagron	Metronidazol	16I19-B04-326151	7
Fagron	Metronidazol	16I19-B04-326152	4
Fagron	Metronidazol	16I19-B04-326155	3
Fagron	Metronidazol	16I19-B04-329159	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazol	16I19-B04-329160	3
Fagron	Metronidazol	16I19-B04-329161	1
Fagron	Metronidazol	16I19-B04-329162	1
Fagron	Metronidazol	16I19-B04-329163	1
Fagron	Metronidazol	16I19-B04-329165	1
Fagron	Metronidazol	16I19-B04-329166	1
Fagron	Metronidazol	16I19-B04-329167	2
Fagron	Metronidazol	16I19-B04-329168	1
Fagron	Metronidazol	16J19B04	1
Fagron	Metronidazol	16J19-B04-326151	1
Fagron	Metronidazol	16J28-B50-329880	1
Fagron	Metronidazol	16L19_B04_326152	1
Fagron	Metronidazol	16l19-B04-326150	1
Fagron	Metronidazol	16l19-B04-329160	1
Fagron	Metronidazol	16l19-B04-329166	1
Fagron	Metronidazol	17/19-304-329168	1
Fagron	Metronidazol	17058003	1
Fagron	Metronidazol	17058013	1
Fagron	Metronidazol	172939-B01-295547	1
Fagron	Metronidazol	17A30-B01-335193	2
Fagron	Metronidazol	17A30-B0-335193	1
Fagron	Metronidazol	17C10	2
Fagron	Metronidazol	17C10-B04	6
Fagron	Metronidazol	17C-10-B04-338699	1
Fagron	Metronidazol	17C10-B04-338700	2
Fagron	Metronidazol	17C10-B04-338707	4
Fagron	Metronidazol	17C10-B04-346275	7
Fagron	Metronidazol	17c10-b04-346276	2
Fagron	Metronidazol	17C10-B04-346276	11
Fagron	Metronidazol	17C10-B04-346277	5
Fagron	Metronidazol	17C10-B04-346278	1
Fagron	Metronidazol	17C10-B04-346279	2
Fagron	Metronidazol	17C10-B04-346280	1
Fagron	Metronidazol	17C10-B04-355863	2
Fagron	Metronidazol	17C10-B04-355864	1
Fagron	Metronidazol	17C10-B04-355865	3
Fagron	Metronidazol	17C10-B04-355867	1
Fagron	Metronidazol	17C10-Bo4-346276	1
Fagron	Metronidazol	17C20-B04-355868	1
Fagron	Metronidazol	1802007-01	1
Fagron	Metronidazol	1802007-02	1
Fagron	Metronidazol	18026401	1
Fagron	Metronidazol	1807039-01	3
Fagron	Metronidazol	18B28-B50-354847	1
Fagron	Metronidazol	18B28B50354848	1
Fagron	Metronidazol	18B28-B50-354848	1
Fagron	Metronidazol	18B28-B50-354849	2
Fagron	Metronidazol	18B28-B50-354851	1
Fagron	Metronidazol	18B28-B50-354852	4
Fagron	Metronidazol	18B28-B50-3554852	1
Fagron	Metronidazol	1901042-01	1
Fagron	Metronidazol	19G002-B04-362813	1
Fagron	Metronidazol	19G02	1
Fagron	Metronidazol	19G02-B02-362815	1
Fagron	Metronidazol	19G02-B04	9
Fagron	Metronidazol	19G02-B04_362823	1
Fagron	Metronidazol	19G02-B04-362812	1
Fagron	Metronidazol	19G02B04362813	1
Fagron	Metronidazol	19G02-B04-362813	5
Fagron	Metronidazol	19G02B04362814	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazol	19G02-B04-362814	6
Fagron	Metronidazol	19G02-B04-362815	8
Fagron	Metronidazol	19G02-B04-362816	11
Fagron	Metronidazol	19G02-B04-362817	1
Fagron	Metronidazol	19G02-B04-362818	2
Fagron	Metronidazol	19G02-B04-362823	5
Fagron	Metronidazol	19G02-B04-367358	1
Fagron	Metronidazol	19G02-B04-367359	2
Fagron	Metronidazol	19G02-B04-367360	1
Fagron	Metronidazol	19G02-B04-367363	2
Fagron	Metronidazol	19G02-B04-36763	1
Fagron	Metronidazol	19GO2-BO4-362814	1
Fagron	Metronidazol	19119-B04-326154	1
Fagron	Metronidazol	20007-F03-0003	1
Fagron	Metronidazol	20121121	3
Fagron	Metronidazol	20130906F	4
Fagron	Metronidazol	20140131f	1
Fagron	Metronidazol	20140131F	3
Fagron	Metronidazol	20G07_F03-372291	1
Fagron	Metronidazol	20g07-f03	1
Fagron	Metronidazol	20G07-F03	8
Fagron	Metronidazol	20G07-F03_372291	1
Fagron	Metronidazol	20G07F03372286	1
Fagron	Metronidazol	20G07-F03-372286	7
Fagron	Metronidazol	20g07-f03-372287	2
Fagron	Metronidazol	20G07-F03-372287	3
Fagron	Metronidazol	20G07-F03-372288	1
Fagron	Metronidazol	20G07-F03-372290	1
Fagron	Metronidazol	20G07-F03-372291	17
Fagron	Metronidazol	20G07-F3-372288	1
Fagron	Metronidazol	21G29-B02	1
Fagron	Metronidazol	21G29-B02-213325	12
Fagron	Metronidazol	21G29-B02-213328	1
Fagron	Metronidazol	21G29-B02-221569	1
Fagron	Metronidazol	21G29-B02-221570	1
Fagron	Metronidazol	220401M	1
Fagron	Metronidazol	2OG07-FO3-372291	1
Fagron	Metronidazol	3212E01870	1
Fagron	Metronidazol	443-48-1	1
Fagron	Metronidazol	48(17C10-B04-346277	1
Fagron	Metronidazol	601021826	2
Fagron	Metronidazol	601062027	4
Fagron	Metronidazol	601072127	1
Fagron	Metronidazol	603041926	4
Fagron	Metronidazol	604081626	6
Fagron	Metronidazol	605021726	4
Fagron	Metronidazol	606/10072017	1
Fagron	Metronidazol	61021826	1
Fagron	Metronidazol	700837-0008	1
Fagron	Metronidazol	700837-B04-367361	1
Fagron	Metronidazol	9041303	1
Fagron	Metronidazol	B04-3628104	1
Fagron	Metronidazol	B04-3628106	2
Fagron	Metronidazol	B04-3673509	1
Fagron	Metronidazol	F03-3722806	2
Fagron	Metronidazol	F03-3722807	1
Fagron	Metronidazol	F03-3722808	1
Fagron	Metronidazol	Metr23012023	1
Fagron	Metronidazol	PM41	1
Farchemia / Gehe	Metronidazol	15253017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Farchemia S. r. l.	Metronidazol	1609028-01	1
Farchemia S.R.L./ Ca...	Metronidazol	15253032	1
Farchemia/Phönix	Metronidazol	1609028-02	1
Fargon	Metronidazol	13D08-N22	1
Fargon	Metronidazol	14c14-b02-291238	1
Fargon	Metronidazol	19G02-B04-367360	1
Fargon	Metronidazol	21G29-B02-213325	1
Fiebig	Metronidazol	16089235	1
Fiebig	Metronidazol	17058005	1
Fiebig	Metronidazol	17058027	1
Fiebig	Metronidazol	17290504	2
Fiebig	Metronidazol	17290506	1
Fiebig	Metronidazol	17290507	1
Fiebig	Metronidazol	17290517	2
Fiebig	Metronidazol	17290527	1
Fiebig	Metronidazol	17290532	1
Fiebig	Metronidazol	b04-3673509	1
Fiebig	Metronidazol	B04-3673509	1
Fischer/Gehe	Metronidazol	15A20-B07-308525	1
Frago/Noweda	Metronidazol	16I19-B04-329163	1
Fragon/Jenne	Metronidazol	19Go2-B04-367359	1
Gatt-Koller	Metronidazol	3728/11162017	1
Gatt-Koller	Metronidazol	497/03151015	1
Gatt-Koller	Metronidazol	497/03151515	1
Gatt-Koller	Metronidazol	497/03154015	1
Gatt-Koller	Metronidazol	606293914	1
GEHE 11.06.2014	Metronidazol	1307002-01	1
Gehe 23.11.18	Metronidazol	1706022-02	1
Gehe am 04.02.14	Metronidazol	1212030-01	2
Gehe amax	Metronidazol	17058012	1
Gehe amax	Metronidazol	17290506	1
Gehe amax	Metronidazol	17290507	2
Gehe amax	Metronidazol	17290533	1
Gehe amax	Metronidazol	1807039-03	1
Gehe amax	Metronidazol	19000516002	1
Gehe amax	Metronidazol	1908028-02	1
Gehe Rostock	Metronidazol	1906012-01	1
Gehe	Metronidazol	10368318	1
Gehe	Metronidazol	1112028-02	1
Gehe	Metronidazol	12110415	1
Gehe	Metronidazol	12110422	1
Gehe	Metronidazol	1307002-01	1
Gehe	Metronidazol	1307002-02	1
Gehe	Metronidazol	140700301	1
Gehe	Metronidazol	1407003-01	2
Gehe	Metronidazol	1505024-01	1
Gehe	Metronidazol	15215108	1
Gehe	Metronidazol	15253017	1
Gehe	Metronidazol	15253026	1
Gehe	Metronidazol	15253032	1
GEHE	Metronidazol	15253032	1
GEHE	Metronidazol	16089216	1
GEHE	Metronidazol	16089229	1
Gehe	Metronidazol	16H15-B50-326734	1
GEHE	Metronidazol	17058013	1
GEHE	Metronidazol	17058015	1
Gehe	Metronidazol	17058016	2
Gehe	Metronidazol	17058019	1
Gehe	Metronidazol	1707008	1
Gehe	Metronidazol	17290506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Metronidazol	17290518	1
Gehe	Metronidazol	1802007-01	1
Gehe	Metronidazol	19000516006	1
Gehe	Metronidazol	19000516008	1
Gehe	Metronidazol	190102003	1
Gehe	Metronidazol	19G02-B04-362813	2
Gehe	Metronidazol	20004568009	1
Gehe	Metronidazol	2005029-02	1
Gehe	Metronidazol	2007002-01	1
Gehe	Metronidazol	2007002-02	1
Gehe	Metronidazol	20140131F	1
Gehe	Metronidazol	21002293020	1
GEHE	Metronidazol	22002266007	1
Gehe	Metronidazol	22002266008	1
Gehe	Metronidazol	220631-01	1
Gehe	Metronidazol	60106207	1
Gehe	Metronidazol	F03-3722806	2
Gehe01/2018	Metronidazol	14C14-B02-291237	1
Geilenkirchen	Metronidazol	13214018	1
Geilenkirchen	Metronidazol	16089222	1
Geilenkirchen	Metronidazol	1807039-03	1
GH: ...	Metronidazol	17290503	1
GUMO	Metronidazol	2007002-01	1
GUMO	Metronidazol	2007002-02	3
Hedinger/Noweda	Metronidazol	166089220	1
Henry Lamotte	Metronidazol	1212001-02	1
Herberata Arzneimittel	Metronidazol	15253024I-02082016	1
Hubei Hongyuan	Metronidazol	140700301	1
Ichthyol Gesellschaft	Metronidazol	13095005	1
Ichthyol/ALH	Metronidazol	1609028-02	1
Infectopharm / Alliance	Metronidazol	18B28-B50-354849	1
Jenne	Metronidazol	21002293006	1
Jenne	Metronidazol	22002266002	1
Jenne	Metronidazol	22002266008	1
Jenne	Metronidazol	24000389003	1
Kehr	Metronidazol	17058003	1
Kehr	Metronidazol	17290512	1
Kehr	Metronidazol	2007002-02	1
Kehr	Metronidazol	21002293020	1
Kehr	Metronidazol	2207001-01	1
Klosterring	Metronidazol	16089235	1
krieger	Metronidazol	19010203	1
Kuerzel	Metronidazol	1307002-02	1
L10	Metronidazol	1807039-01	4
L12	Metronidazol	1609028-01	1
L12	Metronidazol	1609028-02	1
L30	Metronidazol	16089224	2
Laborch.Apolda/Gehe	Metronidazol	17C10_B04_346278	1
Noweda /Cealo	Metronidazol	19000516016	1
Noweda 19.12.22 EK 6,37	Metronidazol	21002293014	2
Noweda 27.11.2019	Metronidazol	19010211	1
Noweda/Wepa	Metronidazol	13214017	1
Noweda	Metronidazol	11319818	1
Noweda	Metronidazol	12110404	1
Noweda	Metronidazol	12339501	1
Noweda	Metronidazol	12G04-N15	1
Noweda	Metronidazol	13095012	1
Noweda	Metronidazol	13214025	1
Noweda	Metronidazol	1407003-01	2
Noweda	Metronidazol	1505024-03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Metronidazol	160902802	1
Noweda	Metronidazol	1619-B04-329166	1
Noweda	Metronidazol	1701039-01	1
Noweda	Metronidazol	17058004	2
Noweda	Metronidazol	17058005	2
Noweda	Metronidazol	17058013	1
Noweda	Metronidazol	17058014	2
Noweda	Metronidazol	1706022-01	1
Noweda	Metronidazol	1707008-01	2
Noweda	Metronidazol	17290518	1
Noweda	Metronidazol	17290519	1
Noweda	Metronidazol	17290526	1
Noweda	Metronidazol	17290532	1
Noweda	Metronidazol	1807039-02	1
Noweda	Metronidazol	1807039-03	1
Noweda	Metronidazol	19000516019	1
Noweda	Metronidazol	19010212	1
Noweda	Metronidazol	19G02-B04-362814	1
Noweda	Metronidazol	20004568015	1
Noweda	Metronidazol	200700201	1
Noweda	Metronidazol	2007002-01	3
Noweda	Metronidazol	2007002-02	2
noweda	Metronidazol	2100223016	1
Noweda	Metronidazol	21002293016	1
Noweda	Metronidazol	21002293017	1
Noweda	Metronidazol	21002293019	1
Noweda	Metronidazol	21002293020	1
Noweda	Metronidazol	22002266004	2
Noweda	Metronidazol	22002266006	1
Noweda	Metronidazol	2206031-01	2
Noweda	Metronidazol	2207001-01	1
Noweda	Metronidazol	2308004-01	1
Otto Fischar GmbH&Co KG	Metronidazol	17058017	1
Phoenix 11.09.13	Metronidazol	12L17-N11	1
Phoenix 11.05.2017 6,59EUR	Metronidazol	16089220	1
Phoenix 12.10.2016 6,63EUR	Metronidazol	15253027	1
Phoenix 15.05.18 6,52EUR	Metronidazol	17058017	1
Phoenix 4.3.2019	Metronidazol	17290526	1
Phoenix/Cealo	Metronidazol	17058016/0818E-0187	1
Phoenix	Metronidazol		1
Phoenix	Metronidazol	121203002	1
Phoenix	Metronidazol	15253032	1
Phoenix	Metronidazol	16089201	1
Phoenix	Metronidazol	16089224	1
Phoenix	Metronidazol	17058002	1
Phoenix	Metronidazol	17058013	1
Phoenix	Metronidazol	17058026	1
Phoenix	Metronidazol	17058027	1
Phoenix	Metronidazol	17290517	1
Phoenix	Metronidazol	17290527	2
Phoenix	Metronidazol	19010202	2
Phoenix	Metronidazol	19010216	1
phoenix	Metronidazol	1908028-02	2
Phoenix	Metronidazol	20004568009	1
Phoenix	Metronidazol	200490406	1
Phoenix	Metronidazol	21002293020	2
Phoenix	Metronidazol	22002266002	2
Phoenix	Metronidazol	3403	1
Phönix Gotha	Metronidazol	13214017	1
Phönix Gotha	Metronidazol	17058018	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix/ Corden Pharm...	Metronidazol	17290518	1
Phönix	Metronidazol	1109030-03	1
Phönix	Metronidazol	121203001	1
Phönix	Metronidazol	12L17-N11	1
Phönix	Metronidazol	13214017	2
Phönix	Metronidazol	13J21-N07	1
Phönix	Metronidazol	15253018	1
phönix	Metronidazol	15253026	1
Phönix	Metronidazol	16089212	1
Phönix	Metronidazol	16089223	1
Phonix	Metronidazol	1612013-01	1
Phönix	Metronidazol	1701039-01	1
Phönix	Metronidazol	17058003	1
Phönix	Metronidazol	17058005	1
PHÖNIX	Metronidazol	17058011	3
Phönix	Metronidazol	17058016	1
Phönix	Metronidazol	1707008-01	1
Phönix	Metronidazol	172905070	1
Phönix	Metronidazol	17290527	1
Phönix	Metronidazol	17290532	1
Phönix	Metronidazol	18026401	1
Phönix	Metronidazol	1807039-01	2
Phönix	Metronidazol	19000516010	2
Phönix	Metronidazol	19010210	1
Phönix	Metronidazol	19010214	1
Phönix	Metronidazol	200700201	1
Phönix	Metronidazol	2007002-01	1
Phönix	Metronidazol	20G07-F03-372286	1
Phönix	Metronidazol	21002293020	2
Phönix	Metronidazol	22002266008	1
Phönix	Metronidazol	2200226606	1
Phönix	Metronidazol	22602266006	1
Phönix	Metronidazol	3179	1
PHÖNIX	Metronidazol	601062027	1
Phönix	Metronidazol	Mez5	1
Phönix_13.12.2018	Metronidazol	17290518	1
Pohlpharma/Noweda	Metronidazol	601062027	3
Polpharma Pharmaceut...	Metronidazol	16I19-B04-326151	1
Polpharma/Noweda	Metronidazol	603041926	1
Reichelt	Metronidazol	17058013	1
Röntgen	Metronidazol	1906012-01	1
Röntgen	Metronidazol	F190012	1
Sana	Metronidazol	19010210	1
Sanacorp 27.10.15	Metronidazol	15A20-B07-303298	1
Sanacorp 02.03.15	Metronidazol	13214009	1
Sanacorp	Metronidazol		1
Sanacorp	Metronidazol	12110422	1
Sanacorp	Metronidazol	12339519	1
Sanacorp	Metronidazol	12G04-N15	1
Sanacorp	Metronidazol	13095002	1
Sanacorp	Metronidazol	16G02-B04-367358	1
Sanacorp	Metronidazol	16I19-B04-329159	1
Sanacorp	Metronidazol	16I19-B04-329160	1
Sanacorp	Metronidazol	1701039-01	1
Sanacorp	Metronidazol	17058002	1
Sanacorp	Metronidazol	17058014	1
Sanacorp	Metronidazol	17058018	1
Sanacorp	Metronidazol	1707008-01	2
Sanacorp	Metronidazol	17290512	1
Sanacorp	Metronidazol	17290518	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Metronidazol	17290525	1
Sanacorp	Metronidazol	17290526	1
Sanacorp	Metronidazol	17290533	2
Sanacorp	Metronidazol	17C10-B04-338707	1
Sanacorp	Metronidazol	17C10-B04-346280	2
Sanacorp	Metronidazol	19000516003	2
Sanacorp	Metronidazol	19010201	1
Sanacorp	Metronidazol	19010211	1
Sanacorp	Metronidazol	1906012-01	1
Sanacorp	Metronidazol	20004568003	2
Sanacorp	Metronidazol	20004568008	1
sanacorp	Metronidazol	200700201	1
Sanacorp	Metronidazol	20G07-F03	2
Sanacorp	Metronidazol	20G07-F03-372286	1
Sanacorp	Metronidazol	21002293020	1
Sanacorp	Metronidazol	21G29-B02-213325	1
Sanacorp	Metronidazol	22002266008	2
Sanacorp	Metronidazol	2206031-01	2
Sanacorp	Metronidazol	39/AKD18	1
Sanacorp	Metronidazol	39/AKD6	1
Sanacorp	Metronidazol	39AKD15	1
Sanacorp	Metronidazol	601021826	1
Sanacorp	Metronidazol	605021726	1
Sanacorp	Metronidazol	F200019	1
Spangro 28.05.2014	Metronidazol	13/10-N03	1
Spangropharm	Metronidazol	11319818	1
synthetisch	Metronidazol	2007002-02	1
test	Metronidazol		1
vdl	Metronidazol	12110421	1
WE Alliance Healthca…	Metronidazol	19010201	1
WEPA/Gehe	Metronidazol	20180515-04P	1

- 230 612 spectra from 1515 *Apo-Ident* customers from a total of 48 491 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metronidazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metronidazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	1130	0	200 954
Type C	0	5323	132	230 612

The substance/substance group *Metronidazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4690 %)
Type C	100.0000 % (> 99.9007 %)	97.5802 % (> 97.5252 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20857	21881	7,92	132,19
21212	22472	7,57	130,07
21213	22472	6,59	129,63
21356	21881	5,39	132,59
21360	22472	4,69	132,37
21881	21881	0,00	131,61
22472	22472	0,00	131,94
22835	22472	2,65	131,90
25330	25330	0,00	127,64
25565	25565	0,00	131,61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Minoxidil**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20879-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Minoxidil; Minoxidilum

Special notes

When selecting the *Minoxidil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Minoxidil	10	20	571

Second-stage model

For differentiation of the substance/substance group *Minoxidil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Minoxidil* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	70,75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Minoxidil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Minoxidil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Minoxidil	13039501	20879	40	20130306
Caelo	Minoxidil	14093701	21359	40	20140428
Caelo	Minoxidil	14093701	21361	40	20140428
Euro OTC	Minoxidil	1311038-01	21630	59	AR-15-FG-007848-01
Euro OTC	Minoxidil	1411006-01	21912	60	20141210
Euro OTC	Minoxidil	1509035	21933	60	20151016*
Euro OTC	Minoxidil	1602013	22365	60	20160225*
Euro OTC	Minoxidil	1612011	22982	40	20170130*
Euro OTC	Minoxidil	2004030	25162	40	20200528*
Euro OTC	Minoxidil	2109021	25888	50	20211104*
Euro OTC	Minoxidil	2109021	25888SI	50	20211104*
Euro OTC	Minoxidil	2209016	26337	40	20221005*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 579 spectra of 12 reference samples from the substance/substance group *Minoxidil*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 383 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1480 spectra of 35 reference samples from the substance/substance group *Minoxidil*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Minoxidil	172278	23816	40
Caelo	Minoxidil	191957	24758	40
Caelo	Minoxidil	20001705	25613	40
Caelo	Minoxidil	23001171	26845	40
Caelo	Minoxidil	24002249	27436	40
Caelo	Minoxidil	24002248	27441	40
Euro OTC	Minoxidil	1607007	22688	40
Euro OTC	Minoxidil	1705008	23437	40
Euro OTC	Minoxidil	1710043	23896	40
Euro OTC	Minoxidil	1803004	24062	40
Euro OTC	Minoxidil	1807018-01	24190	40
Euro OTC	Minoxidil	1901005	24489	40
Euro OTC	Minoxidil	1907025	24803	40
Euro OTC	Minoxidil	2001035	25120	40
Euro OTC	Minoxidil	2008040	25334	40
Euro OTC	Minoxidil	2008039	25343	40
Euro OTC	Minoxidil	2109018	25866	50
Euro OTC	Minoxidil	2209017	26349	40
Euro OTC	Minoxidil	2311021	27342	40
Fagron	Minoxidil	22C01-B03-218964	26139	40
Caelo	Minoxidil	20001705	25613SI	40
Caelo	Minoxidil	23001171	26845SI	40
Caelo	Minoxidil	24002249	27436SI	40
Caelo	Minoxidil	24002248	27441SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Minoxidil	1411006-01	21912SI†	60
Euro OTC	Minoxidil	1509035	21933SI†	60
Euro OTC	Minoxidil	1602013	22365SI†	60
Euro OTC	Minoxidil	1612011	22982SI†	40
Euro OTC	Minoxidil	2008040	25334SI	40
Euro OTC	Minoxidil	2008039	25343SI	40
Euro OTC	Minoxidil	2109018	25866SI	50
Euro OTC	Minoxidil	2209016	26337SI†	40
Euro OTC	Minoxidil	2209017	26349SI	40
Euro OTC	Minoxidil	2311021	27342SI	40
Fagron	Minoxidil	22C01-B03-218964	26139SI	40

- 200 604 spectra from a total of 4020 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3373 spectra from 805 *Apo-Ident* customers from 594 batches from the substance/substance group *Minoxidil*.
- Among them are spectra of independent samples from 541 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Minoxidil	21002063017	1
	Minoxidil	21002063019	1
	Minoxidil	21002063022	4
	Minoxidil	2109018-01	1
	Minoxidil	2109021-01	2
	Minoxidil	2109021-02	5
	Minoxidil	22000546001	3
	Minoxidil	22000546005	1
	Minoxidil	22000546006	3
	Minoxidil	22000546008	4
	Minoxidil	22000546010	6
	Minoxidil	22003	1
	Minoxidil	2209016	1
	Minoxidil	2209016-01	22
	Minoxidil	2209017-01	9
	Minoxidil	2209017-03	1
	Minoxidil	22C01-B03-220935	1
	Minoxidil	22c01-b03-220944	1
	Minoxidil	22I05-B06	1
	Minoxidil	22I05-B06-225227	1
	Minoxidil	22I05-B06-225228	1
	Minoxidil	23001171003	2
	Minoxidil	2300325300	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Minoxidil	23003253001	2
	Minoxidil	23003253003	1
	Minoxidil	23A18-B03-227781	1
	Minoxidil	23D27-B04-230212	1
	Minoxidil	Minox280623	1
/Noweda	Minoxidil	181498002	1
A.H.D	Minoxidil	1210056-01	1
AHC 14.08.13 EK40,14	Minoxidil	1210056-02	1
AHD/Euro	Minoxidil	171004301	1
AHD	Minoxidil	1210056-01	1
AHD	Minoxidil	1311038-01	1
AHD	Minoxidil	1504013-02	1
AHD	Minoxidil	15230812	1
AHD	Minoxidil	18149801	1
AHD	Minoxidil	1907025-02	1
AHD	Minoxidil	200803901	1
AHD	Minoxidil	24B28-B11-236694	1
Alliance health	Minoxidil	1411006-01	3
Alliance Healthc. 15...	Minoxidil	1203035-03	1
Alliance Healthcare	Minoxidil	1210056-01	1
Alliance Healthcare	Minoxidil	1210056-02	1
Alliance Healthcare	Minoxidil	21002063013	1
Alliance	Minoxidil	21002063017	1
Alliance	Minoxidil	2109018-01	1
Alliance	Minoxidil	23A18-B03-227781	1
Anzag 14.11.12 ek:40,14	Minoxidil	120303501	1
Anzag 18.10.12 ek:40,14	Minoxidil	1203035-01	1
Anzag	Minoxidil	1112024-02	1
Anzag	Minoxidil	13E13-N10	1
Anzag	Minoxidil	14234505	1
anzag	Minoxidil	1504013-02	1
api-ident	Minoxidil	1710043-01	2
apo-ident.	Minoxidil	1607007-07	1
Apo-ident	Minoxidil	190102502	1
apomix	Minoxidil	1504013-02	1
apomix	Minoxidil	1602013-01	1
Audor Pharma	Minoxidil		51
Audor Pharma	Minoxidil	20008039-01	1
Audor Pharma	Minoxidil	414E-02844	1
Audor Pharma	Minoxidil	8/14M	1
Audor Pharma	Minoxidil	AP001/16M	7
Audor Pharma	Minoxidil	AP006/13M	2
Audor Pharma	Minoxidil	AP006/17M	5
Audor Pharma	Minoxidil	AP007/15M	4
Audor Pharma	Minoxidil	AP008/14M	6
Audor Pharma	Minoxidil	AP010/12M	5
Audor Pharma	Minoxidil	AP011/16M	2
Audor Pharma	Minoxidil	AP012/16M	4
Audor Pharma	Minoxidil	AP012/16M/5270	1
Audor Pharma	Minoxidil	AP016/15M	8
Audor Pharma	Minoxidil	AP-016/15M	1
Audor Pharma	Minoxidil	AP020/11M	3
Audor Pharma	Minoxidil	AP088/14M	1
Audor Pharma	Minoxidil	APK007	1
Audor Pharma	Minoxidil	APK0071/16/04/065-1M	1
Bombastus	Minoxidil	1112024-03	1
Bombastus	Minoxidil	1705008-01	2
Bombastus	Minoxidil	1710043-01	1
Bombastus	Minoxidil	4/13	1
Caelo	Minoxidil		11

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	1070318/17227803	1
Caelo	Minoxidil	1112024-01	1
Caelo	Minoxidil	11150207	1
Caelo	Minoxidil	11150209	1
Caelo	Minoxidil	11302003	1
Caelo	Minoxidil	11302005	1
Caelo	Minoxidil	11e17-n07	1
Caelo	Minoxidil	11K11-n09	1
Caelo	Minoxidil	12023901	2
Caelo	Minoxidil	12023902	1
Caelo	Minoxidil	12023907	4
Caelo	Minoxidil	12023908	1
Caelo	Minoxidil	1203035	1
Caelo	Minoxidil	1203035-01	1
Caelo	Minoxidil	121005601	1
Caelo	Minoxidil	1210056-01	2
Caelo	Minoxidil	1210056-02	3
Caelo	Minoxidil	12273703	2
Caelo	Minoxidil	12273704	3
Caelo	Minoxidil	12273710	1
Caelo	Minoxidil	12H07-N03	4
Caelo	Minoxidil	13/23-N07	1
Caelo	Minoxidil	13039501	7
Caelo	Minoxidil	13039503	3
Caelo	Minoxidil	130402901	1
Caelo	Minoxidil	130402902	1
Caelo	Minoxidil	1309501	1
Caelo	Minoxidil	1311038-01	2
Caelo	Minoxidil	13179501	2
Caelo	Minoxidil	13179501-3467312121	1
Caelo	Minoxidil	13179502	5
Caelo	Minoxidil	13179503	6
Caelo	Minoxidil	13179504	2
Caelo	Minoxidil	13179507	3
Caelo	Minoxidil	13373106	1
Caelo	Minoxidil	13E13-N10	1
Caelo	Minoxidil	13I23-N07	2
Caelo	Minoxidil	13K04B05290380	1
Caelo	Minoxidil	1405028-01	2
Caelo	Minoxidil	14062018-RQ-A	1
Caelo	Minoxidil	14093702	2
Caelo	Minoxidil	14093703	4
Caelo	Minoxidil	14093706	3
Caelo	Minoxidil	14093707	1
Caelo	Minoxidil	1411006-01	2
Caelo	Minoxidil	14234502	2
Caelo	Minoxidil	14234505	5
Caelo	Minoxidil	14234509	3
Caelo	Minoxidil	14L03-B02-301431	1
Caelo	Minoxidil	150401301	1
Caelo	Minoxidil	1504013-01	5
Caelo	Minoxidil	1504013-02	1
Caelo	Minoxidil	1509035	1
Caelo	Minoxidil	1509035-01	3
Caelo	Minoxidil	1520002455	1
Caelo	Minoxidil	15230802	4
Caelo	Minoxidil	15230803	3
Caelo	Minoxidil	15230804	7
Caelo	Minoxidil	15230805	2
Caelo	Minoxidil	15230806	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	15230811	5
Caelo	Minoxidil	15230812	1
Caelo	Minoxidil	15436024	1
Caelo	Minoxidil	15436201	8
Caelo	Minoxidil	15436202	7
Caelo	Minoxidil	15436202/1060217	1
Caelo	Minoxidil	15436204	3
Caelo	Minoxidil	15436404	4
Caelo	Minoxidil	15436406	5
Caelo	Minoxidil	15436408	8
Caelo	Minoxidil	15436412	2
Caelo	Minoxidil	15436414	6
Caelo	Minoxidil	15436415	2
Caelo	Minoxidil	15E19-B06-308182	1
Caelo	Minoxidil	15E19-B06-308183	1
Caelo	Minoxidil	15E19-B06-309180	1
Caelo	Minoxidil	15H07-B03-317340	1
Caelo	Minoxidil	15K17-B05-318240	1
Caelo	Minoxidil	15K17-B05-318692	1
Caelo	Minoxidil	15K17-B06-321926	1
Caelo	Minoxidil	15k17-b06-324965	1
Caelo	Minoxidil	160013-01	1
Caelo	Minoxidil	1602013-01	9
Caelo	Minoxidil	160201302	2
Caelo	Minoxidil	1602013-02	4
Caelo	Minoxidil	1607007-01	4
Caelo	Minoxidil	160707-01	1
Caelo	Minoxidil	161201101	2
Caelo	Minoxidil	1612011-01	8
Caelo	Minoxidil	16J24-B04-328218	1
Caelo	Minoxidil	16J24-B05-331128	1
Caelo	Minoxidil	16J24-B05-332092	1
Caelo	Minoxidil	170043-01	1
Caelo	Minoxidil	17011602	1
Caelo	Minoxidil	170500801	5
Caelo	Minoxidil	1705008-01	7
Caelo	Minoxidil	1710043-01	8
Caelo	Minoxidil	17227801	18
Caelo	Minoxidil	17227803	20
Caelo	Minoxidil	17228703	1
Caelo	Minoxidil	17H08-B06-341377	1
Caelo	Minoxidil	17H08-B06-342282	1
Caelo	Minoxidil	18016103	2
Caelo	Minoxidil	18016104	3
Caelo	Minoxidil	18016107	5
Caelo	Minoxidil	18016109	8
Caelo	Minoxidil	18016112	2
Caelo	Minoxidil	1803004-001	1
Caelo	Minoxidil	1803004-01	3
Caelo	Minoxidil	1807018_01	1
Caelo	Minoxidil	180701801	1
Caelo	Minoxidil	1807018-01	8
Caelo	Minoxidil	181498001	1
Caelo	Minoxidil	181498002	2
Caelo	Minoxidil	18149801	7
Caelo	Minoxidil	18149802	18
Caelo	Minoxidil	18149805	4
Caelo	Minoxidil	18149810	7
Caelo	Minoxidil	18149811	1
Caelo	Minoxidil	18149813	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	18149815	17
Caelo	Minoxidil	18159810	1
Caelo	Minoxidil	187018-01	1
Caelo	Minoxidil	18C20-B01-35661844	1
Caelo	Minoxidil	18C27-B01	1
Caelo	Minoxidil	1901005-01	3
Caelo	Minoxidil	190702501	1
Caelo	Minoxidil	1907025-01	1
Caelo	Minoxidil	190702502	1
Caelo	Minoxidil	19149810	1
Caelo	Minoxidil	19157002	1
Caelo	Minoxidil	191957002	7
Caelo	Minoxidil	191957003	7
Caelo	Minoxidil	191957004	5
Caelo	Minoxidil	191957007	7
Caelo	Minoxidil	191957010	6
Caelo	Minoxidil	200001705004	1
Caelo	Minoxidil	2000040	1
Caelo	Minoxidil	20001705004	4
Caelo	Minoxidil	20004048001	2
Caelo	Minoxidil	20004048003	9
Caelo	Minoxidil	20004048005	5
Caelo	Minoxidil	20004048008	2
Caelo	Minoxidil	20004048009	7
Caelo	Minoxidil	20004048012	2
Caelo	Minoxidil	2000408012	1
Caelo	Minoxidil	200804001	1
Caelo	Minoxidil	2008040-01	1
Caelo	Minoxidil	20151112-5	1
Caelo	Minoxidil	20160211-1	1
Caelo	Minoxidil	21002063001	9
Caelo	Minoxidil	21002063003	8
Caelo	Minoxidil	21002063005	2
Caelo	Minoxidil	21002063006	8
Caelo	Minoxidil	21002063009	2
Caelo	Minoxidil	21002063011	4
Caelo	Minoxidil	21002063012	3
Caelo	Minoxidil	21002063013	4
Caelo	Minoxidil	21002063015	2
Caelo	Minoxidil	21002063017	4
Caelo	Minoxidil	21002063018	12
Caelo	Minoxidil	210902101	1
Caelo	Minoxidil	22000546005	2
Caelo	Minoxidil	22000546008	2
Caelo	Minoxidil	22031402	1
Caelo	Minoxidil	2827	1
Caelo	Minoxidil	2905047-01	1
Caelo	Minoxidil	3013M-02844	1
Caelo	Minoxidil	31051305	1
Caelo	Minoxidil	41/17	1
Caelo	Minoxidil	5081502	1
Caelo	Minoxidil	5217M-02844	1
Caelo	Minoxidil	8719	1
Caelo	Minoxidil	AP006/17M	1
Caelo	Minoxidil	AP011/16M	1
Caelo	Minoxidil	K0071/16/04/065	1
Caesaer/Jenne	Minoxidil	18016103	1
Caesar & Loretz GmbH...	Minoxidil	14093702	1
Caesar & Loretz GmbH...	Minoxidil	14234505	1
Caesar & Loretz GmbH...	Minoxidil	18149813	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/AHD	Minoxidil	20004048009	1
Caesar & Loretz GmbH...	Minoxidil	20004048005	1
Caesar & Loretz GmbH...	Minoxidil	20004048008	1
Caesar & Loretz GmbH...	Minoxidil	191957002	1
Caesar & Loretz GmbH...	Minoxidil	20004048012	1
Caesar & Loretz GmbH...	Minoxidil	21002063006	3
Caesar & Loretz GmbH...	Minoxidil	21002063004	3
Caesar & Loretz GmbH	Minoxidil		1
Caesar & Loretz GmbH	Minoxidil	13039501	1
Caesar & Loretz GmbH	Minoxidil	17227803	1
Caesar & Loretz GmbH	Minoxidil	181498002	1
Caesar & Loretz GmbH	Minoxidil	18149801	1
Caesar & Loretz GmbH	Minoxidil	18149802	6
Caesar & Loretz GmbH	Minoxidil	18149810	2
Caesar & Loretz GmbH	Minoxidil	18149813	3
Caesar & Loretz GmbH	Minoxidil	18149815	5
Caesar & Loretz GmbH	Minoxidil	191957002	4
Caesar & Loretz GmbH	Minoxidil	191957004	3
Caesar & Loretz GmbH	Minoxidil	191957007	5
Caesar & Loretz GmbH	Minoxidil	191957010	3
Caesar & Loretz GmbH	Minoxidil	20001705004	7
Caesar & Loretz GmbH	Minoxidil	20004048003	2
Caesar & Loretz GmbH	Minoxidil	20004048005	7
Caesar & Loretz GmbH	Minoxidil	20004048008	4
Caesar & Loretz GmbH	Minoxidil	20004048009	3
Caesar & Loretz GmbH	Minoxidil	20004048012	1
Caesar & Loretz GmbH	Minoxidil	21000123003	1
Caesar & Loretz GmbH	Minoxidil	21002063001	3
Caesar & Loretz GmbH	Minoxidil	21002063003	2
Caesar & Loretz GmbH	Minoxidil	21002063004	1
Caesar & Loretz GmbH	Minoxidil	21002063005	2
Caesar & Loretz GmbH	Minoxidil	21002063006	2
Caesar & Loretz GmbH	Minoxidil	21002063011	2
Caesar & Loretz GmbH	Minoxidil	21002063012	3
Caesar & Loretz GmbH	Minoxidil	21002063017	1
Caesar & Loretz GmbH	Minoxidil	21002063018	1
Caesar & Loretz GmbH	Minoxidil	22000546001	1
Caesar & Loretz GmbH	Minoxidil	22000546005	1
Caesar & Loretz GmbH	Minoxidil	22000546008	1
Caesar & Loretz	Minoxidil	15436414	1
Caleo/ Noweda	Minoxidil	18016104	1
Doppeleiche Apotheke	Minoxidil	13E13-N10	2
Dr. Wolff / Sanacorp	Minoxidil	1901005-01	2
EuRho / 2	Minoxidil	2004030-01	1
EuRho / AHD 19.08.21...	Minoxidil	2008040-01	2
EuRho / Noweda	Minoxidil	1304029-02	1
EuRho / Sanacorp	Minoxidil	1710043-01	1
EuRho /Sanacorp	Minoxidil	2008040-01	2
EuRho/ Alliance	Minoxidil	1705008-01	1
EuRho/ Alliance	Minoxidil	1901005-01	1
EuRho/ Noweda	Minoxidil	1807018-01	1
EuRho/ NOWEDA	Minoxidil	1807018-01	1
EuRho/ Phoenix	Minoxidil	2109018-01	2
EuRho/Anzag	Minoxidil	1411006-01	1
EuRho/Fiebig	Minoxidil	1411006-01	1
EuRho/Gehe	Minoxidil	2008039-01	2
EuRho/Gehe	Minoxidil	2109018-01	1
EuRho/Kehr	Minoxidil	1803004-01	2
EuRho/Kehr	Minoxidil	30/17	1
EuRho/Noweda	Minoxidil	1607007-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Noweda	Minoxidil	1710043-01	2
Eurho/Phönix	Minoxidil	2004030-01	1
Eurho/Phönix	Minoxidil	2008039-01	1
EuRho/Sanacorp	Minoxidil	17050008-01	1
EuRho/Sanacorp	Minoxidil	1803004-01	2
EuRho/Sanacorp	Minoxidil	1901005-01	1
EuRho/Sanacorp	Minoxidil	1907025-01	2
EuRho/Sanacorp	Minoxidil	2004030-01	1
EuRho	Minoxidil	1105030-02	1
EuRho	Minoxidil	1108039-02	2
EuRho	Minoxidil	1602013-02	1
eurho	Minoxidil	1705008-01	1
EuRho	Minoxidil	1705008-01	1
EuRho	Minoxidil	1710043-01	3
Eurho	Minoxidil	1803004-01	2
EuRho	Minoxidil	1803004-01	1
EuRho	Minoxidil	1901005-01	3
EuRho	Minoxidil	2004030-01	5
EuRho	Minoxidil	2008039-01	2
euRho	Minoxidil	2008040-01	1
EuRho	Minoxidil	2008040-01	1
EuRho	Minoxidil	2109018-01	2
Eurho	Minoxidil	2109021-02	2
Euro OCT / Krieger	Minoxidil	2001035-01	1
Euro OT/Phönix	Minoxidil	1710043-01	1
Euro OTC	Minoxidil		17
Euro OTC	Minoxidil	/18/07/1402	1
Euro OTC	Minoxidil	10/13	1
Euro OTC	Minoxidil	1009042-01	3
Euro OTC	Minoxidil	103004-01	1
Euro OTC	Minoxidil	104029-02	1
Euro OTC	Minoxidil	1102010-02	1
Euro OTC	Minoxidil	1108039-01	1
Euro OTC	Minoxidil	1108039-03	1
Euro OTC	Minoxidil	1112024-01	1
Euro OTC	Minoxidil	1112024-02	5
Euro OTC	Minoxidil	1112024-03	3
Euro OTC	Minoxidil	12/16	2
Euro OTC	Minoxidil	12/17	2
Euro OTC	Minoxidil	1203035	1
Euro OTC	Minoxidil	1203035-01	10
Euro OTC	Minoxidil	1203035-02	6
Euro OTC	Minoxidil	120303503	1
Euro OTC	Minoxidil	1203035-03	11
Euro OTC	Minoxidil	12100056-01	1
Euro OTC	Minoxidil	121005601	1
Euro OTC	Minoxidil	1210056-01	14
Euro OTC	Minoxidil	1210056-02	26
Euro OTC	Minoxidil	13001	1
Euro OTC	Minoxidil	130402901	1
Euro OTC	Minoxidil	1304029-01	16
Euro OTC	Minoxidil	130402902	1
Euro OTC	Minoxidil	1304029-02	15
Euro OTC	Minoxidil	1304029-C2	1
Euro OTC	Minoxidil	131103801	4
Euro OTC	Minoxidil	1311038-01	30
Euro OTC	Minoxidil	13110838-01	1
Euro OTC	Minoxidil	140502801	3
Euro OTC	Minoxidil	1405028-01	29
Euro OTC	Minoxidil	14050281	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	1405028-1	1
Euro OTC	Minoxidil	140528-01	1
Euro OTC	Minoxidil	141100601	5
Euro OTC	Minoxidil	1411006-01	43
Euro OTC	Minoxidil	1411006601	1
Euro OTC	Minoxidil	150401-01	1
Euro OTC	Minoxidil	1504013-01	36
Euro OTC	Minoxidil	1504013-02	27
Euro OTC	Minoxidil	1504013-2	1
Euro OTC	Minoxidil	15081829	1
Euro OTC	Minoxidil	1509035-01	42
Euro OTC	Minoxidil	15436404	1
Euro OTC	Minoxidil	160201301	1
Euro OTC	Minoxidil	1602013-01	44
Euro OTC	Minoxidil	1602013-02	14
Euro OTC	Minoxidil	1602013-1	1
Euro OTC	Minoxidil	1602016-01	1
Euro OTC	Minoxidil	16070007-01	1
Euro OTC	Minoxidil	1607001-01	1
Euro OTC	Minoxidil	1607007	1
Euro OTC	Minoxidil	160700701	3
Euro OTC	Minoxidil	1607007-01	40
Euro OTC	Minoxidil	16112011-01	2
Euro OTC	Minoxidil	16120-01	1
Euro OTC	Minoxidil	161201-01	1
Euro OTC	Minoxidil	1612011	1
Euro OTC	Minoxidil	161201101	2
Euro OTC	Minoxidil	1612011-01	81
Euro OTC	Minoxidil	1612011-011	1
Euro OTC	Minoxidil	16122011_01	1
Euro OTC	Minoxidil	17050008	1
Euro OTC	Minoxidil	1705008_01	1
Euro OTC	Minoxidil	170500801	3
Euro OTC	Minoxidil	1705008-01	57
Euro OTC	Minoxidil	1707018-01	1
Euro OTC	Minoxidil	170703M/1602013-02	1
Euro OTC	Minoxidil	1710043_01	1
Euro OTC	Minoxidil	171004301	9
Euro OTC	Minoxidil	1710043-01	103
Euro OTC	Minoxidil	17100-43-01	1
Euro OTC	Minoxidil	1710043-03	1
Euro OTC	Minoxidil	17H08-B06	1
Euro OTC	Minoxidil	17H08-B06-342282	1
Euro OTC	Minoxidil	17H08-B09-346945	1
Euro OTC	Minoxidil	18030004-01	1
Euro OTC	Minoxidil	1803004	1
Euro OTC	Minoxidil	1803004_01	2
Euro OTC	Minoxidil	180300401	7
Euro OTC	Minoxidil	1803004-01	115
Euro OTC	Minoxidil	180304-01	1
Euro OTC	Minoxidil	1807017-01	1
Euro OTC	Minoxidil	1807018	1
Euro OTC	Minoxidil	180701801	1
Euro OTC	Minoxidil	1807018-01	60
Euro OTC	Minoxidil	1807018-02	3
Euro OTC	Minoxidil	180708-01	1
Euro OTC	Minoxidil	180718-01	1
Euro OTC	Minoxidil	19/15	1
Euro OTC	Minoxidil	19/16	1
Euro OTC	Minoxidil	190100-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	19010005-01	1
Euro OTC	Minoxidil	190100501	3
Euro OTC	Minoxidil	1901005-01	83
Euro OTC	Minoxidil	19011005-01	1
Euro OTC	Minoxidil	1907025	1
Euro OTC	Minoxidil	1907025_01	1
Euro OTC	Minoxidil	190702501	4
Euro OTC	Minoxidil	1907025-01	63
Euro OTC	Minoxidil	190702502	4
Euro OTC	Minoxidil	1907025-02	38
Euro OTC	Minoxidil	1907025-41	1
Euro OTC	Minoxidil	1919	1
Euro OTC	Minoxidil	20004048005	1
Euro OTC	Minoxidil	2000804001	1
Euro OTC	Minoxidil	20008040-01	1
Euro OTC	Minoxidil	2001035-01	23
Euro OTC	Minoxidil	2002312844	1
Euro OTC	Minoxidil	2004020-01	1
Euro OTC	Minoxidil	200403001	9
Euro OTC	Minoxidil	2004030-01	119
Euro OTC	Minoxidil	2004030-1	2
Euro OTC	Minoxidil	20080039-01	1
Euro OTC	Minoxidil	200803901	9
Euro OTC	Minoxidil	2008039-01	95
Euro OTC	Minoxidil	2008040	2
Euro OTC	Minoxidil	2008040_01	2
Euro OTC	Minoxidil	200804001	2
Euro OTC	Minoxidil	2008040-01	108
Euro OTC	Minoxidil	2008040-1	1
Euro OTC	Minoxidil	200840-01	1
Euro OTC	Minoxidil	2091714	1
Euro OTC	Minoxidil	210018-01	1
Euro OTC	Minoxidil	2103021-02	1
Euro OTC	Minoxidil	2109018	1
Euro OTC	Minoxidil	210901801	2
Euro OTC	Minoxidil	2109018-01	69
Euro OTC	Minoxidil	2109021-01	23
Euro OTC	Minoxidil	2109021-02	12
Euro OTC	Minoxidil	210918-01	1
Euro OTC	Minoxidil	210921-02	1
Euro OTC	Minoxidil	2209016-01	4
Euro OTC	Minoxidil	29071402	1
Euro OTC	Minoxidil	4/13	2
Euro OTC	Minoxidil	4004030-01	1
Euro OTC	Minoxidil	6/12	2
Euro OTC	Minoxidil	6614849	1
Euro OTC	Minoxidil	700158	1
Euro Pharm/Gehe	Minoxidil	1901005-01	1
euro pharm	Minoxidil	1590035	1
Euro/ Phönix	Minoxidil	1405028-01	1
EUro/AHD	Minoxidil	1203035-03	2
Euro/Anzag	Minoxidil	150903501	1
Euro/Gehe	Minoxidil	1112024-03	1
Euro/Gehe	Minoxidil	140528-01	1
Euro/Krieger	Minoxidil	1602013-02	1
Euro/Noweda	Minoxidil	1602013-02	1
Euro/Noweda	Minoxidil	1612011-01	1
Euro/Phönix	Minoxidil	161201101	2
Euro/Phönix	Minoxidil	1612011-01	1
Euro/Phönix	Minoxidil	1901005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Phönix	Minoxidil	1901005-01	3
Euro/Phönix	Minoxidil	2001035-01	1
Euro/Phönix	Minoxidil	20044030-01	1
Euro/Phönix	Minoxidil	210901801	2
Euro	Minoxidil	1304029-02	1
Euro	Minoxidil	1504013-01	2
euro	Minoxidil	2008039-01	1
euroct/Gehe	Minoxidil	1304029-01	1
EuRoh/ Gehe	Minoxidil	2008039-01	1
EuRoh	Minoxidil	2008040-01	1
europharm/gehe	Minoxidil	1710043-01	1
Europharm/Sanacorp	Minoxidil	1210056-01	1
EurPS	Minoxidil	1504013-01	2
Faagron/Fiebig 09.04.19	Minoxidil	18c27-B01-354525	1
Fagrin	Minoxidil	15K17-B06-321926	1
Fagron	Minoxidil		2
Fagron	Minoxidil	1/16M	2
Fagron	Minoxidil	11021402	1
Fagron	Minoxidil	11E17-N07	1
Fagron	Minoxidil	11H07-N03	1
Fagron	Minoxidil	11K11-N09	2
Fagron	Minoxidil	120303503	1
Fagron	Minoxidil	1210056-02	1
Fagron	Minoxidil	12A25-N04	4
Fagron	Minoxidil	12C29-N05	4
Fagron	Minoxidil	12C29-N050087/240	1
Fagron	Minoxidil	12C29-N050145/240	1
Fagron	Minoxidil	12H07N03	1
Fagron	Minoxidil	12H07-N03	12
Fagron	Minoxidil	12H07-N030265/432	1
Fagron	Minoxidil	12H07-No3	1
Fagron	Minoxidil	12H07-NO3	1
Fagron	Minoxidil	12HO7-NO3	1
Fagron	Minoxidil	1311038-01	2
Fagron	Minoxidil	13E13N10	1
Fagron	Minoxidil	13E13-N10	9
Fagron	Minoxidil	13H07-NO3	1
Fagron	Minoxidil	13I23-N07	8
Fagron	Minoxidil	13J23N07	2
Fagron	Minoxidil	13J29-B02	1
Fagron	Minoxidil	13K04-B05-0004	1
Fagron	Minoxidil	13K04-B05-290377	6
Fagron	Minoxidil	13K04-B05-290379	2
Fagron	Minoxidil	13K04-B05-290380	3
Fagron	Minoxidil	13123-N07	1
Fagron	Minoxidil	1411006-01	2
Fagron	Minoxidil	1420001962	1
Fagron	Minoxidil	14B04-B07	1
Fagron	Minoxidil	14B04-B07-290883	3
Fagron	Minoxidil	14B04-B07-297364	1
Fagron	Minoxidil	14L03-B02	3
Fagron	Minoxidil	14L03-B02-30129	1
Fagron	Minoxidil	14L03-B02-301428	1
Fagron	Minoxidil	14L03-B02301429	1
Fagron	Minoxidil	14L03-B02-301429	7
Fagron	Minoxidil	14L03-B02-301430	2
Fagron	Minoxidil	14L03-B02-301431	1
Fagron	Minoxidil	14L03-B02301434	1
Fagron	Minoxidil	14L03-B02-301541	1
Fagron	Minoxidil	14L03-Bo2-301430	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	1504013-01	2
Fagron	Minoxidil	1510001251	3
Fagron	Minoxidil	1520000768	2
Fagron	Minoxidil	1520002631	2
Fagron	Minoxidil	15436408	1
Fagron	Minoxidil	15E19-06-308183	1
Fagron	Minoxidil	15E19-B06	1
Fagron	Minoxidil	15E19-B06-308179	1
Fagron	Minoxidil	15e19-b06-308180	1
Fagron	Minoxidil	15E19-B06-308180	5
Fagron	Minoxidil	15E19-B06-308181	6
Fagron	Minoxidil	15E19-B06-308182	5
Fagron	Minoxidil	15E19-B06-308183	6
Fagron	Minoxidil	15E19-B09-308181	1
Fagron	Minoxidil	15E19-B06-308183	1
Fagron	Minoxidil	15F02-B08	1
Fagron	Minoxidil	15F02-B09-312663	2
Fagron	Minoxidil	15H07-B01-313607	1
Fagron	Minoxidil	15H07-B01-314726	2
Fagron	Minoxidil	15K17-B05	1
Fagron	Minoxidil	15K17-B05-318240	2
Fagron	Minoxidil	15K17-B05-318241	2
Fagron	Minoxidil	15K17-B05-318411	2
Fagron	Minoxidil	15K17-B05-318691	4
Fagron	Minoxidil	15K17-B05-318692	1
Fagron	Minoxidil	15K17-B05-320188	3
Fagron	Minoxidil	15K17-B06	1
Fagron	Minoxidil	15K17-B06-321926	5
Fagron	Minoxidil	15K17-B06-321927	3
Fagron	Minoxidil	15K17-B06-321928	2
Fagron	Minoxidil	15k17-b06-324965	1
Fagron	Minoxidil	15K17-B06-324965	3
Fagron	Minoxidil	15K17-B06-325490	3
Fagron	Minoxidil	15K17-B06-325491	2
Fagron	Minoxidil	15K197-B05-318411	1
Fagron	Minoxidil	16/24-B04-328218	1
Fagron	Minoxidil	1612011-01	1
Fagron	Minoxidil	16j24-b04328218	1
Fagron	Minoxidil	16J24-B04-328218	6
Fagron	Minoxidil	16J24-B04-328219	1
Fagron	Minoxidil	16J24-B04-328224	2
Fagron	Minoxidil	16J24-B04-328225	1
Fagron	Minoxidil	16J24-B04-328226	3
Fagron	Minoxidil	16j24-B04-329291	1
Fagron	Minoxidil	16J24-B04-329291	1
Fagron	Minoxidil	16J24-B05	1
Fagron	Minoxidil	16J24-B05-332092	5
Fagron	Minoxidil	16J24-B05-332093	2
Fagron	Minoxidil	1705008-01	2
Fagron	Minoxidil	170612184	1
Fagron	Minoxidil	1722	1
Fagron	Minoxidil	17B22/B02/336689	2
Fagron	Minoxidil	17b22-b01	1
Fagron	Minoxidil	17B22-B01	2
Fagron	Minoxidil	17B22-B01-334447	1
Fagron	Minoxidil	17B22-B01-335427	8
Fagron	Minoxidil	17B22-B02	2
Fagron	Minoxidil	17B22-B02-336689	3
Fagron	Minoxidil	17B22-B02-336690	1
Fagron	Minoxidil	17B22-B02-336700	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	17B22-B02-338766	3
Fagron	Minoxidil	17B22-B02-338767	1
Fagron	Minoxidil	17H08-B06	1
Fagron	Minoxidil	17H08-B06-340512	2
Fagron	Minoxidil	17H08-B06-340514	2
Fagron	Minoxidil	17H08-B06-341376	5
Fagron	Minoxidil	17H08-B06-341377	5
Fagron	Minoxidil	17h08-b06-342282	1
Fagron	Minoxidil	17H08-B09	4
Fagron	Minoxidil	17H08-B09-346945	3
Fagron	Minoxidil	17H08-B09-346947	2
Fagron	Minoxidil	17H08-B09-346948	1
Fagron	Minoxidil	17H08-B09-347482	1
Fagron	Minoxidil	18002	2
Fagron	Minoxidil	18003	1
Fagron	Minoxidil	18004	3
Fagron	Minoxidil	18008	4
Fagron	Minoxidil	1803004-01	2
Fagron	Minoxidil	18C19-B01-348984	4
Fagron	Minoxidil	18C19-B01-348985	2
Fagron	Minoxidil	18C20-B01	4
Fagron	Minoxidil	18C20-b01-351844	1
Fagron	Minoxidil	18C20-B01-351844	4
Fagron	Minoxidil	18C20-B01-352113	1
Fagron	Minoxidil	18C20-B01-352116	2
Fagron	Minoxidil	18C20-B01-352629	5
Fagron	Minoxidil	18C20-B01-352702	5
Fagron	Minoxidil	18C20-B01-352874	1
Fagron	Minoxidil	18C27-B01-354524	3
Fagron	Minoxidil	18C27-B01-354525	7
Fagron	Minoxidil	18C27-B01-354782	1
Fagron	Minoxidil	18C-B01-352116	1
Fagron	Minoxidil	18L19-B05-356595	6
Fagron	Minoxidil	18L19-BO5-356595	1
Fagron	Minoxidil	19002	2
Fagron	Minoxidil	19003	5
Fagron	Minoxidil	19004	1
Fagron	Minoxidil	1901005-01	1
Fagron	Minoxidil	1907025-01	2
Fagron	Minoxidil	19b18-b06-191023	1
Fagron	Minoxidil	19B21-190615	1
Fagron	Minoxidil	19B21-B07	1
Fagron	Minoxidil	19B21-B07-190615	9
Fagron	Minoxidil	19B21-B07-190616	2
Fagron	Minoxidil	19B21-B07-190617	6
Fagron	Minoxidil	19B21-B07-190618	9
Fagron	Minoxidil	19B21-B07-190628	1
Fagron	Minoxidil	19B21-B07-190661	1
Fagron	Minoxidil	19B21-B07-19618	1
Fagron	Minoxidil	19E28-B12	3
Fagron	Minoxidil	19E28-B12_193438	1
Fagron	Minoxidil	19E28-B12-1934308	1
Fagron	Minoxidil	19E28-B12-193438	9
Fagron	Minoxidil	19E28-B12-193440	1
Fagron	Minoxidil	19E28-B12-193447	1
Fagron	Minoxidil	19E28-B12-193449	4
Fagron	Minoxidil	19g22-B02	1
Fagron	Minoxidil	19G22-B02	2
Fagron	Minoxidil	19G22-B02-193448	10
Fagron	Minoxidil	19G22-B02-1934939	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	19G22-B02-193448	1
Fagron	Minoxidil	2/16M	4
Fagron	Minoxidil	2008039-01	1
Fagron	Minoxidil	20A07-B02-197710	1
Fagron	Minoxidil	20A07-b02-197718	1
Fagron	Minoxidil	20A07-B02-197718	1
Fagron	Minoxidil	20A07-B02-197719	2
Fagron	Minoxidil	20A07-B02-197720	3
Fagron	Minoxidil	20A15-B99	1
Fagron	Minoxidil	20A15-B99_196663	1
Fagron	Minoxidil	20A15-B99-196663	8
Fagron	Minoxidil	20A15-B99-196664	1
Fagron	Minoxidil	20A15-B99-196667	2
Fagron	Minoxidil	20A15-B99-196668	1
Fagron	Minoxidil	20D27-B11	1
Fagron	Minoxidil	20D27-B11-201184	3
Fagron	Minoxidil	20D27-B11-201247	2
Fagron	Minoxidil	20D27-B11-201331	2
Fagron	Minoxidil	20K05-B03-202207	2
Fagron	Minoxidil	21001	1
Fagron	Minoxidil	21B02-B13	2
Fagron	Minoxidil	21B02-B13-2153704	1
Fagron	Minoxidil	21B02-B13-215374	2
Fagron	Minoxidil	21B11_B18_203082	1
Fagron	Minoxidil	21B11-B18	1
Fagron	Minoxidil	21B11-B18-203081	3
Fagron	Minoxidil	21B11-B18-203082	1
Fagron	Minoxidil	21B11-B18-203084	2
Fagron	Minoxidil	21B11-B20-210128	6
Fagron	Minoxidil	21B16-B15-220936	1
Fagron	Minoxidil	21B16B15220943	1
Fagron	Minoxidil	21F07-B05-215378	5
Fagron	Minoxidil	21F07-B06	1
Fagron	Minoxidil	21F07-B06-213152	1
Fagron	Minoxidil	21F07-B07-0004	1
Fagron	Minoxidil	21F07-B07-216774	4
Fagron	Minoxidil	21F07-B07-216859	2
Fagron	Minoxidil	21F07-B07-216892	1
Fagron	Minoxidil	21F07-B07-216984	1
Fagron	Minoxidil	21J06-B05-213146	3
Fagron	Minoxidil	21JO6-B05-213146	1
Fagron	Minoxidil	22C01_b03-21915	1
Fagron	Minoxidil	22C01-B03	1
Fagron	Minoxidil	22C01-B03-218964	4
Fagron	Minoxidil	22C01-B03-220935	1
Fagron	Minoxidil	26111302	1
Fagron	Minoxidil	27081301	1
Fagron	Minoxidil	2OD27-B11-201218	1
Fagron	Minoxidil	321926	1
Fagron	Minoxidil	4110I-02844	1
Fagron	Minoxidil	5/17M	1
Fagron	Minoxidil	612212844	1
Fagron	Minoxidil	7/13	1
Fagron	Minoxidil	B02-1934309	1
Fagron	Minoxidil	B05-215378	2
Fagron	Minoxidil	B11-2011804	1
Fagron	Minoxidil	B12-1934409	1
Fagron	Minoxidil	B13-2131407	1
Fagron	Minoxidil	B18-2030801	2
Fagron	Minoxidil	B99-1966607	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fargon	Minoxidil	20A15-B97-197717	1
Fargon	Minoxidil	21B11-B20-210128	1
Fiebig ek: 36.06EUR 31.0812	Minoxidil	111202403	1
Fiebig	Minoxidil	1509035-01	1
Fiebig	Minoxidil	1607007-01	1
Fiebig	Minoxidil	1612011-01	1
Fiebig	Minoxidil	1705008-01	1
Fiebig	Minoxidil	171004301	1
Fiebig	Minoxidil	1710043-01	1
Fiebig	Minoxidil	1807017-01	1
Fiebig	Minoxidil	1901005-01	1
Fiebig	Minoxidil	1907025	1
Fiebig	Minoxidil	1907025-02	1
Fiebig	Minoxidil	2004030-01	1
Fragon	Minoxidil	20K05-B03-202207	1
Gatt-Koller	Minoxidil	1803103	2
Gehe / EuRho	Minoxidil	1803004-01	1
GEHE/ EuRho	Minoxidil	2109021-02	2
Gehe/Euro	Minoxidil	150903501	1
Gehe/EuRoh	Minoxidil	1907025-02	1
Gehe	Minoxidil		4
Gehe	Minoxidil	1405028-01	1
Gehe	Minoxidil	15436201	1
Gehe	Minoxidil	15436404	1
Gehe	Minoxidil	15436406	1
Gehe	Minoxidil	15436414	1
Gehe	Minoxidil	15K17-B06-321926	1
Gehe	Minoxidil	1602013-01	2
Gehe	Minoxidil	1612011-01	1
Gehe	Minoxidil	1705008-01	1
Gehe	Minoxidil	1710043-01	1
Gehe	Minoxidil	17227803	2
Gehe	Minoxidil	17H08-B06-341376	1
Gehe	Minoxidil	1803004-01	1
Gehe	Minoxidil	1807018-01	1
Gehe	Minoxidil	1901005-01	1
Gehe	Minoxidil	1907025-01	2
GEHE	Minoxidil	1907025-01	1
Gehe	Minoxidil	1907025-02	1
Gehe	Minoxidil	2004030-01	2
GEHE	Minoxidil	2109021-01	1
GEHE	Minoxidil	2209016-01	4
Gehe	Minoxidil	2209017-01	4
Gehe	Minoxidil	23H25-B13-234500	2
Gehe	Minoxidil	AP006/13M	1
Geibo	Minoxidil	1705008-01	1
Geilenkirchen	Minoxidil	14234505	1
Hedinger/Fiebig	Minoxidil	1612011-01	1
Hedinger/Noweda	Minoxidil	15436414	1
Hedinger/Sanacorp	Minoxidil	12C29-N05	1
Hedinger	Minoxidil	14B04-B07	2
Ichthyol/Noweda	Minoxidil	17117803	1
Ichthyol-Gesellschaft	Minoxidil	1311038-01	1
Icrom / Gehe	Minoxidil	20A15-B99-1966607	1
Icrom /Oberlinden-Ap...	Minoxidil	1/14	1
Icrom S.P.A./Sanacorp	Minoxidil	1907025-01	1
Icrom S.P.A./Sanacorp	Minoxidil	1907025-02	1
icrom spa	Minoxidil	511v	1
ICROM/Gehe	Minoxidil	12/17	1
Icrom/Gehe	Minoxidil	1602013-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
ICROM	Minoxidil	6/12	1
Jenne	Minoxidil	17H08-B06-341377	2
Jenne	Minoxidil	B99-1966007	1
Jenne	Minoxidil	P2019/93	1
Kehr	Minoxidil	1705008-01	1
Kehr	Minoxidil	1803004-01	1
Krieger	Minoxidil	171004301	1
Krieger	Minoxidil	21B11-B20-210128	1
Kumar Cigan	Minoxidil	2004030-01	1
Kumar Organic Produc...	Minoxidil		1
Kumar Organics Products	Minoxidil	2001035-01	1
Kumar organics	Minoxidil	200804001	1
Kumar/Phoenix	Minoxidil		1
Laborchemie Apolda G...	Minoxidil	1803004-01	2
Moweda	Minoxidil	2311021-01	1
Noweda/ Infecto Pharm	Minoxidil	1607007-01	1
Noweda/Euro	Minoxidil	20080440-01	1
Noweda	Minoxidil	14093703	1
Noweda	Minoxidil	15K17-B05-320189	2
Noweda	Minoxidil	1705008-01	1
Noweda	Minoxidil	1710043-01	3
Noweda	Minoxidil	1803004-01	2
Noweda	Minoxidil	18149801	1
Noweda	Minoxidil	18149802	2
Noweda	Minoxidil	1901005-01	1
Noweda	Minoxidil	1907025-01	4
Noweda	Minoxidil	191957003	1
Noweda	Minoxidil	19E28-B12-193438	1
Noweda	Minoxidil	2004030-01	4
Noweda	Minoxidil	20040301	1
Noweda	Minoxidil	21002063012	1
Noweda	Minoxidil	210901801	1
Noweda	Minoxidil	2109018-01	1
Noweda	Minoxidil	2109021-02	1
Noweda	Minoxidil	22000546010	1
Oberlinden Apotheke	Minoxidil	5-13	1
Olon Spa	Minoxidil	15K17-B06-321926	1
Ph.Eur.10.0/Gehe	Minoxidil	2001035-01	1
phoenix /EuRho	Minoxidil	2004030-01	3
PhOENIX 19.03.2012	Minoxidil	1311038-01	2
Phoenix	Minoxidil	1602013-02	1
Phoenix	Minoxidil	16J25-B05-332092	1
Phoenix	Minoxidil	2004030-01	1
Phoenix	Minoxidil	2008039-01	1
Phoenix	Minoxidil	2008040-01	1
Phoenix	Minoxidil	2109021-01	1
Phoenix	Minoxidil	21B02-B13-215374	1
Phoenix	Minoxidil	24B28-B11-236694	2
Phoenix	Minoxidil	3057	1
Phoenix	Minoxidil	3399	1
Phönix /euro	Minoxidil	170500801	2
Phönix/EuRho	Minoxidil	1710043-01	2
phönix	Minoxidil		1
Phönix	Minoxidil	1112024-03	1
Phönix	Minoxidil	1203035-02	1
Phönix	Minoxidil	1304029-01	1
Phönix	Minoxidil	1504013-01	1
phönix	Minoxidil	1509035-01	1
phönix	Minoxidil	1602013-01	3
Phönix	Minoxidil	1602013-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
phönix	Minoxidil	1612011-01	2
Phönix	Minoxidil	1612011-01	1
Phönix	Minoxidil	170043-01	1
Phönix	Minoxidil	1705008-01	1
PHÖNIX	Minoxidil	1705008-01	2
Phönix	Minoxidil	18016109	1
Phönix	Minoxidil	18149815	1
Phönix	Minoxidil	1901005-01	1
Phönix	Minoxidil	1907025-01	2
Phönix	Minoxidil	19B21-B07-190661	1
Phönix	Minoxidil	2001030-01	1
Phönix	Minoxidil	2004030-01	5
PHÖNIX	Minoxidil	2004030-01	1
Phönix	Minoxidil	2008040-01	2
Phönix	Minoxidil	201062710	1
Phönix	Minoxidil	2109018-01	1
Phönix	Minoxidil	2209016-01	1
Phonix	Minoxidil	2311021-01	1
PHÖNIX	Minoxidil	CB2109018-01	1
Sana Eurho 11.11.19 ...	Minoxidil	1907025-01	1
sanacorb	Minoxidil	1612011-01	1
Sanacorp, 81,00EUR, 27.1.17	Minoxidil	1607007-01	1
Sanacorp/EuRho	Minoxidil	2001035-01	1
Sanacorp	Minoxidil	120056-01	1
Sanacorp	Minoxidil	1203035-01	1
Sanacorp	Minoxidil	1210056-01	1
Sanacorp	Minoxidil	1210056-02	2
Sanacorp	Minoxidil	1304029-02	3
Sanacorp	Minoxidil	13179501	2
Sanacorp	Minoxidil	13179502	2
Sanacorp	Minoxidil	13179507	1
sanacorp	Minoxidil	13K04-B05-290379	1
sanacorp	Minoxidil	1405028-01	1
Sanacorp	Minoxidil	140502801	1
Sanacorp	Minoxidil	1405028-01	1
Sanacorp	Minoxidil	14093701	1
Sanacorp	Minoxidil	14093702	1
Sanacorp	Minoxidil	1411006-01	1
Sanacorp	Minoxidil	1504013-01	1
Sanacorp	Minoxidil	1612011-01	1
Sanacorp	Minoxidil	180300401	1
Sanacorp	Minoxidil	1907025-01	1
Sanacorp	Minoxidil	191957010	1
Sanacorp	Minoxidil	2008040	1
Sanacorp	Minoxidil	2008040-01	2
Sanacorp	Minoxidil	20D27-B11-201218	1
Sanacorp	Minoxidil	21002063022	4
Sanacorp	Minoxidil	2109021-02	1
Sanacorp	Minoxidil	21b02-b13-215377	1
Sanacorp	Minoxidil	21B11-B18-203084	2
Sanacorp	Minoxidil	21F07-B05-215378	2
Sanacorp	Minoxidil	22000546001	1
Spangro 1.10.19	Minoxidil	16J24-B04-328224	1
Spangro 25.1.2014	Minoxidil	13/23-N07	1
Th. Geyer	Minoxidil	1602013-01	1
Vdl 14.07.14	Minoxidil	1311038-01	1
VDL;81,0EUR;21.05.15	Minoxidil	1411006-01	1

- 232 694 spectra from 1515 *Apo-Ident* customers from a total of 48 677 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Minoxidil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Minoxidil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	579	0	152 383
Type B	0	1478	2	200 604
Type C	0	3362	11	232 694

The substance/substance group *Minoxidil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9637 %)
Type B	100.0000 % (> 99.9912 %)	99.8649 % (> 99.6622 %)
Type C	100.0000 % (> 99.9007 %)	99.6739 % (> 99.5849 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20879	21630	7,45	195,66
21359	21630	5,53	195,22
21361	21630	5,06	195,77
21630	21630	0,00	195,41
21912	21933	5,08	196,67
21933	21933	0,00	193,02
22365	22365	0,00	198,76
22982	22982	0,00	200,92
25162	25162	0,00	197,43
25888	25888	0,00	198,96
26337	26337	0,00	200,20

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Minoxidil sulfato**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006688-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Minoxidil sulfato; Minoxidil sulfate

Special notes

When selecting the *Minoxidil sulfato* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Minoxidil sulfato	2	1	0

Second-stage model

For differentiation of the substance/substance group *Minoxidil sulfato* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Minoxidil sulfato* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	92,77	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Minoxidil sulfato* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Minoxidil sulfato*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Minoxidil sulfate	01801022407017	BR20044	40	20241230*
Fagron	Minoxidil sulfate	01801022405015	BR20046	40	20240930*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Minoxidil sulfato*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 4 reference samples from the substance/substance group *Minoxidil sulfato*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Minoxidil sulfate	01801022406016	BR20045	40
Fagron	Minoxidil sulfate	01801022407017	BR20044SI†	20
Fagron	Minoxidil sulfate	01801022406016	BR20045SI	20
Fagron	Minoxidil sulfate	01801022405015	BR20046SI†	20

- 201 984 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Minoxidil sulfato*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Minoxidil sulfato* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

relevant spectra of the various substances were compared with *Minoxidil sulfato* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	100	0	201 984
Type C	0	0	0	236 067

The substance/substance group *Minoxidil sulfato* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
BR20044	BR20044	0,00	130,11
BR20046	BR20046	0,00	126,21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mio-inositol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20420-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mio-inositol; myo-Inositolum

Special notes

When selecting the *Mio-inositol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mio-inositol	3	1	6

Second-stage model

For differentiation of the substance/substance group *Mio-inositol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mio-inositol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	76,22	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mio-inositol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mio-inositol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Mio-inositol	1206032-01	21280	40	20120814
Fagron	Mio-inositol	13D15-B40-328250	23405	40	20140812
Fagron	Mio-inositol	13D15-B40-328250	23406	40	AR-17-FG-016393-01
Fagron	Mio-inositol	23D12-B07-223058	26730	40	20230517
Fagron	Mio-inositol	23D12-B07-223058	26730SI	20	20230517

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Mio-inositol*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 782 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Mio-inositol*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Mio-inositol	18A03-B04-344527	23999	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Mio-inositol*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Mio-inositol	L1609025-01	1
Euro OTC	Mio-inositol	130400901	1
Euro OTC	Mio-inositol	1304009-01	1
Euro OTC	Mio-inositol	1609025-01	1
Euro OTC	Mio-inositol	L2010021-01	1
Fagron	Mio-inositol	L13090200	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mio-inositol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mio-inositol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	40	0	202 044
Type C	0	6	0	236 061

The substance/substance group *Mio-inositol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21280	23406	5,70	185,03
23405	23406	3,07	176,22
23406	23406	0,00	176,57
26730	23406	6,59	184,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Monoestearatos**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20691-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Monoestearatos; Glyceroli monostearas 40–55; Glyceroli monostearates 60; Glyceroli monostearates emulsificantes; Monoestearato de glicerila 40-55; Monoestearato de glicerila 60; Monoestearato de glicerila emulsificante; Monoestearato de glicerol 40-55; Monoestearato de glicerol 60; Monoestearato de glicerol, emulsionante; Monoestearato de sorbitano; Sorbitan stearate; Sorbitani stearas; Span 60

Special notes

When selecting the *Monoestearatos* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Monoestearatos	37	19	141

Second-stage model

For differentiation of the substance/substance group *Monoestearatos* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Monoestearatos* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cetostearyl alcohol (type A), emuls…	48,60	–
Álcool emulsificante não iônico	52,15	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Monoestearatos* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Monoestearatos*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Monoestearato de glicerol…	12105705	20691	80	20120424
Caelo	Monoestearato de glicerol…	12105720	20867	40	20120424
Caelo	Monoestearato de glicerol…	14099903	21446	60	AR-15-FG-000732-02
Caelo	Monoestearato de glicerol…	154450	22464	60	20160225*
Caelo	Monoestearato de glicerol…	20002884	25620	40	20200916*
Caelo	Monoestearato de glicerol…	22000532	26018	40	20220331*
Caelo	Monoestearato de glicerol…	23000431	26729	40	20230526*
Caelo	Monoestearato de glicerol…	23000431	26729SI	20	20230526*
Fagron	Monoestearato de glicerol…	14C12-B40-292622	21545	60	20140404
Fagron	Monoestearato de glicerol…	15E13-B03-305532	22277	60	20150703
Caelo	Monoestearato de glicerol 60	13109304	21093	40	1407633
Caelo	Monoestearato de glicerol 60	13232604	21437	60	1504599
Caelo	Monoestearato de glicerol 60	15286302	21982	60	20150911
Caelo	Monoestearato de glicerol 60	15286302	22320	60	AR-16-FG-009226-01
Caelo	Monoestearato de glicerol 60	16233804	23188	40	10052
Caelo	Monoestearato de glicerol 60	180683	24025	40	20180430*
Caelo	Monoestearato de glicerol 60	182462	24371	40	20181008*
Caelo	Monoestearato de glicerol 60	190547	24673	40	20190423*
Caelo	Monoestearato de glicerol 60	192857002	25385	40	20191216
Caelo	Monoestearato de glicerol 60	21003001	26004	40	20211109*
Caelo	Monoestearato de glicerol 60	21003001	26004SI	30	20211109*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Monoestearato de glicerol 60	22003434	26728	40	20230213*
Caelo	Monoestearato de glicerol 60	22003434	26728SI	20	20230213*
Caelo	Monoestearato de glicerol 60	24001839	27316	40	20240829*
Caelo	Monoestearato de glicerol 60	24001839	27316SI	20	20240829*
Caelo	Monoestearato de glicerol...	12210401	20751	80	1407214
Caelo	Monoestearato de glicerol...	12210401	20783	40	20120726
Caelo	Monoestearato de glicerol...	14240607	21576	60	1412120
Caelo	Monoestearato de glicerol...	14240607	21585	60	20140815
Caelo	Monoestearato de glicerol...	161646	22623	40	20160727*
Caelo	Monoestearato de glicerol...	16030301	22667	40	20160204
Caelo	Monoestearato de glicerol...	21000650	25618	40	20210310*
Caelo	Monoestearato de glicerol...	21002557002	26235	40	20210920
Caelo	Monoestearato de glicerol...	21002557002	26235SI	20	20210920
Caelo	Monoestearato de glicerol...	22003075	26480	40	20221121*
Caelo	Monoestearato de glicerol...	22003075	26480SI	20	20221121*
Caelo	Monoestearato de glicerol...	23002137	26958	40	20230829*
Caelo	Monoestearato de glicerol...	23002137	26958SI	20	20230829*
Caelo	Monoestearato de sorbitano	12274801	20828	40	20120924
Caelo	Monoestearato de sorbitano	162352	22764	40	20160826*
Caelo	Monoestearato de sorbitano	17030805	23706	40	20170210
Caelo	Monoestearato de sorbitano	172564	23831	40	20171027*
Caelo	Monoestearato de sorbitano	192928	25094	40	20191122*
Caelo	Monoestearato de sorbitano	20002274	25564	40	20201009*
Caelo	Monoestearato de sorbitano	22002437	26369	40	20220819*
Caelo	Monoestearato de sorbitano	22002437	26369SI	20	20220819*
Caelo	Monoestearato de sorbitano	24000967	27257	40	20240529*
Fagron	Monoestearato de sorbitano	14J07-B02-299399	21885	60	AR-16-FG-004368-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2050 spectra of 48 reference samples from the substance/substance group *Monoestearatos*. These samples are listed above in the *calibration samples* section. The reference samples come from 37 different batches.
- 150 912 spectra from a total of 2805 batches from further 482 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1210 spectra of 29 reference samples from the substance/substance group *Monoestearatos*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Monoestearato de glicerol…	180447	24267	40
Caelo	Monoestearato de glicerol…	190794	24709	40
Caelo	Monoestearato de glicerol…	191186	24713	40
Caelo	Monoestearato de glicerol…	24000632	27255	40
Caelo	Monoestearato de glicerol 60	11272902	20677	80
Caelo	Monoestearato de glicerol 60	162338	22646	40
Caelo	Monoestearato de glicerol 60	20002478	25505	40
Caelo	Monoestearato de glicerol…	14308310	21993	60
Caelo	Monoestearato de glicerol…	172585	23822	40
Fagron	Monoestearato de glicerol…	11I15-N09	20746	80
Fagron	Monoestearato de glicerol…	12B14-N10	20786	40
Caelo	Monoestearato de sorbitano	171781	23622	40
Caelo	Monoestearato de sorbitano	180432	24021	40
Caelo	Monoestearato de sorbitano	183125	24377	40
Caelo	Monoestearato de sorbitano	192168	24900	40
Caelo	Monoestearato de sorbitano	21001797	25807	50
Caelo	Monoestearato de sorbitano	21004159	25991	40
Caelo	Monoestearato de sorbitano	24002443	27435	40
Fagron	Monoestearato de sorbitano	11I26-N09	20736	40
Caelo	Monoestearato de glicerol…	22000532	26018SI†	10
Caelo	Monoestearato de glicerol…	24000632	27255SI	20
Caelo	Monoestearato de glicerol 60	162338	22741	40
Caelo	Monoestearato de glicerol 60	162338	22742	40
Caelo	Monoestearato de glicerol 60	162338	22743	40
Caelo	Monoestearato de glicerol 60	162338	22744	40
Caelo	Monoestearato de glicerol…	14308310	22278	60
Caelo	Monoestearato de glicerol…	14308310	22341	60
Caelo	Monoestearato de sorbitano	21004159	25991SI	10
Caelo	Monoestearato de sorbitano	24000967	27257SI†	20

- 200 874 spectra from a total of 4024 batches from further 839 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 447 spectra from 226 *Apo-Ident* customers from 148 batches from the substance/substance group *Monoestearatos*.
- Among them are spectra of independent samples from 136 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Supplier	Substance	Batch	Spectra
	Monoestearato de glicerol...	22000532003	1
	Monoestearato de glicerol 60	22001891001	1
	Monoestearato de glicerol 60	22001891004	1
	Monoestearato de sorbitano	22002437005	1
	Monoestearato de sorbitano	22002437008	1
	Monoestearato de sorbitano	22003955002	1
	Monoestearato de sorbitano	23000412001	1
	Monoestearato de glicerol 60	23001269003	1
ALH	Monoestearato de sorbitano	16235202	1
Alliance	Monoestearato de sorbitano	21004159001	1
Anzag	Monoestearato de glicerol 60	12180502	1
anzag	Monoestearato de sorbitano	14195	1
Audor Pharma	Monoestearato de glicerol 60	13232604	1
Bombastus	Monoestearato de glicerol...	18044701	1
Caelo	Monoestearato de glicerol 60		1
Caelo	Monoestearato de glicerol...	11079308	1
Caelo	Monoestearato de glicerol 60	12001001	1
Caelo	Monoestearato de glicerol...	12105704	1
Caelo	Monoestearato de glicerol...	12105729	1
Caelo	Monoestearato de glicerol 60	12180502	1
Caelo	Monoestearato de sorbitano	12274807	1
Caelo	Monoestearato de sorbitano	12274813	2
Caelo	Monoestearato de glicerol 60	13018201	3
Caelo	Monoestearato de glicerol 60	1301821	1
Caelo	Monoestearato de glicerol 60	13109304	9
Caelo	Monoestearato de glicerol...	13109402	1
Caelo	Monoestearato de glicerol...	13109405	2
Caelo	Monoestearato de glicerol...	13109410	1
Caelo	Monoestearato de glicerol...	131156602	1
Caelo	Monoestearato de glicerol...	13156601	2
Caelo	Monoestearato de sorbitano	13209409	2
Caelo	Monoestearato de sorbitano	13209410	1
Caelo	Monoestearato de sorbitano	13209417	3
Caelo	Monoestearato de sorbitano	13209418	2
Caelo	Monoestearato de sorbitano	13209419	3
Caelo	Monoestearato de glicerol...	13221303	2
Caelo	Monoestearato de glicerol...	13221308	1
Caelo	Monoestearato de glicerol 60	13232604	3
Caelo	Monoestearato de sorbitano	13B19-N01	1
Caelo	Monoestearato de glicerol 60	14012002	4
Caelo	Monoestearato de sorbitano	14038504	1
Caelo	Monoestearato de sorbitano	14038510	1
Caelo	Monoestearato de sorbitano	14038511	2
Caelo	Monoestearato de glicerol...	14169710	1
Caelo	Monoestearato de glicerol...	1420607	1
Caelo	Monoestearato de sorbitano	14218803	3
Caelo	Monoestearato de sorbitano	14218804	1
Caelo	Monoestearato de sorbitano	14218808	5
Caelo	Monoestearato de sorbitano	14218809	1
Caelo	Monoestearato de glicerol...	14240605	2
Caelo	Monoestearato de glicerol...	14240607	1
Caelo	Monoestearato de glicerol...	14240611	1
Caelo	Monoestearato de glicerol...	14308310	4
Caelo	Monoestearato de glicerol...	14359407	2
Caelo	Monoestearato de sorbitano	14372803	1
Caelo	Monoestearato de glicerol 60	15009203	13
Caelo	Monoestearato de glicerol...	15130501	1
Caelo	Monoestearato de glicerol...	15280902	1
Caelo	Monoestearato de glicerol...	15280903	2
Caelo	Monoestearato de glicerol...	15280904	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Monoestearato de glicerol...	15280912	1
Caelo	Monoestearato de glicerol 60	15286302	4
Caelo	Monoestearato de glicerol 60	15286307	2
Caelo	Monoestearato de glicerol 60	15286308	4
Caelo	Monoestearato de sorbitano	15300302	7
Caelo	Monoestearato de sorbitano	15300308	5
Caelo	Monoestearato de sorbitano	15415202	9
Caelo	Monoestearato de glicerol...	15445007	6
Caelo	Monoestearato de glicerol...	15445010	1
Caelo	Monoestearato de glicerol...	15445011	1
Caelo	Monoestearato de glicerol...	15445014	2
Caelo	Monoestearato de glicerol...	16030301	3
Caelo	Monoestearato de glicerol...	16030304	2
Caelo	Monoestearato de glicerol...	16164604	1
Caelo	Monoestearato de glicerol...	16164606	1
Caelo	Monoestearato de glicerol 60	16233802	2
Caelo	Monoestearato de glicerol 60	16233804	6
Caelo	Monoestearato de sorbitano	16235202	5
Caelo	Monoestearato de sorbitano	16235207	11
Caelo	Monoestearato de sorbitano	17030805	7
Caelo	Monoestearato de sorbitano	17030806	2
Caelo	Monoestearato de glicerol 60	17061703	5
Caelo	Monoestearato de glicerol 60	17167803	7
Caelo	Monoestearato de glicerol 60	17167804	6
Caelo	Monoestearato de sorbitano	17178102	21
Caelo	Monoestearato de glicerol...	17258501	2
Caelo	Monoestearato de glicerol...	17258505	2
Caelo	Monoestearato de sorbitano	17345402	6
Caelo	Monoestearato de sorbitano	17345403P-181005-2	1
Caelo	Monoestearato de sorbitano	17345403P-181227-8	1
Caelo	Monoestearato de glicerol...	18044701	2
Caelo	Monoestearato de glicerol...	18044702	1
Caelo	Monoestearato de glicerol 60	18068303	3
Caelo	Monoestearato de sorbitano	18204705	8
Caelo	Monoestearato de glicerol 60	18246203	3
Caelo	Monoestearato de glicerol 60	18246207	5
Caelo	Monoestearato de sorbitano	18312504P-190502-1	1
Caelo	Monoestearato de sorbitano	18312504P-190627-8	1
Caelo	Monoestearato de sorbitano	18312507P-191230-1	1
Caelo	Monoestearato de glicerol...	18328702	4
Caelo	Monoestearato de glicerol...	18328705	2
Caelo	Monoestearato de glicerol...	18334601	1
Caelo	Monoestearato de glicerol...	18334601P-190405-2	1
Caelo	Monoestearato de glicerol 60	19054702	13
Caelo	Monoestearato de glicerol...	190794001	2
Caelo	Monoestearato de glicerol...	19079401	8
Caelo	Monoestearato de sorbitano	19101301	1
Caelo	Monoestearato de sorbitano	19101302P-190718-8	1
Caelo	Monoestearato de sorbitano	19101302P-190926-7	1
Caelo	Monoestearato de sorbitano	19101305	4
Caelo	Monoestearato de sorbitano	19101306P-200326-8	1
Caelo	Monoestearato de sorbitano	19101306P-200709-5	1
Caelo	Monoestearato de glicerol 60	191258003	7
Caelo	Monoestearato de glicerol...	192039002	6
Caelo	Monoestearato de glicerol...	192039003	1
Caelo	Monoestearato de sorbitano	192168003	1
Caelo	Monoestearato de glicerol 60	192857001	1
Caelo	Monoestearato de glicerol 60	192857002	2
Caelo	Monoestearato de sorbitano	20001211004	1
Caelo	Monoestearato de glicerol...	20001564002	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Monoestearato de glicerol 60	20002478004	1
Caelo	Monoestearato de glicerol...	200028840001	1
Caelo	Monoestearato de glicerol...	20002884001	1
Caelo	Monoestearato de glicerol...	20002884002	1
Caelo	Monoestearato de sorbitano	20003871004	1
Caelo	Monoestearato de glicerol 60	21000650001	6
Caelo	Monoestearato de glicerol...	21000650004	1
Caelo	Monoestearato de glicerol...	2100065001	1
Caelo	Monoestearato de glicerol 60	21001621002	5
Caelo	Monoestearato de glicerol 60	21001621004	3
Caelo	Monoestearato de sorbitano	21001797001	3
Caelo	Monoestearato de glicerol...	21002557002	1
Caelo	Monoestearato de glicerol 60	21003001004	7
Caelo	Monoestearato de sorbitano	21004159001	1
Caelo	Monoestearato de sorbitano	22001545003	1
Caelo	Monoestearato de sorbitano	26031507	1
Caelo	Monoestearato de glicerol 60	7035059	1
Caesar & Loretz GmbH...	Monoestearato de glicerol...	21000650001	1
Caesar & Loretz GmbH...	Monoestearato de sorbitano	22001545003	1
Caesar & Loretz GmbH/Gehe	Monoestearato de sorbitano	20003871007	1
Caesar & Loretz GmbH/Kehr	Monoestearato de sorbitano	20003871004	1
Caesar & Loretz GmbH...	Monoestearato de glicerol 60	19054702	1
Caesar & Loretz GmbH...	Monoestearato de sorbitano	18204705	1
Caesar & Loretz GmbH...	Monoestearato de glicerol 60	18246203	1
Caesar & Loretz GmbH/Sa	Monoestearato de glicerol...	19079404	1
Caesar & Loretz GmbH/Sa	Monoestearato de glicerol...	20001564002	1
Caesar & Loretz GmbH...	Monoestearato de sorbitano	19101301	1
Caesar & Loretz GmbH...	Monoestearato de sorbitano	21001797001	1
Caesar & Loretz GmbH	Monoestearato de glicerol 60	18068303	1
Caesar & Loretz GmbH	Monoestearato de sorbitano	18204705	1
Caesar & Loretz GmbH	Monoestearato de glicerol...	18328702	1
Caesar & Loretz GmbH	Monoestearato de glicerol...	18328705	1
Caesar & Loretz GmbH	Monoestearato de glicerol 60	19054702	3
Caesar & Loretz GmbH	Monoestearato de glicerol...	19079401	2
Caesar & Loretz GmbH	Monoestearato de sorbitano	19101305	1
Caesar & Loretz GmbH	Monoestearato de glicerol 60	191258003	2
Caesar & Loretz GmbH	Monoestearato de glicerol...	192039002	1
Caesar & Loretz GmbH	Monoestearato de sorbitano	192168003	2
Caesar & Loretz GmbH	Monoestearato de glicerol 60	192857002	3
Caesar & Loretz GmbH	Monoestearato de sorbitano	20001211004	1
Caesar & Loretz GmbH	Monoestearato de glicerol...	20003935003	1
Caesar & Loretz GmbH	Monoestearato de glicerol 60	21001621002	1
Caesar & Loretz GmbH	Monoestearato de glicerol 60	21001621004	1
Caesar & Loretz GmbH	Monoestearato de glicerol...	21002557002	4
Caesar & Loretz GmbH	Monoestearato de glicerol...	22000532003	1
Caesar & Loretz GmbH	Monoestearato de glicerol...	22000532004	1
Caesar & Loretz GmbH	Monoestearato de sorbitano	22001545003	1
Caesar & Loretz GmbH	Monoestearato de sorbitano	22002437005	1
Caesar & Loretz Hild...	Monoestearato de sorbitano	19101305	1
Caesar & Loretz/Noweda	Monoestearato de glicerol 60	15009203	1
Caesar u Loretz	Monoestearato de glicerol 60	13109304	1
Caesar u Loretz	Monoestearato de glicerol 60	14012002	1
Caesar&Loretz GmbH/Gehe	Monoestearato de glicerol...	17258505	1
Caesar/Noweda	Monoestearato de glicerol 60	13109304	1
Caesar/Noweda	Monoestearato de glicerol...	13221311	2
cealo sanacorp	Monoestearato de glicerol 60	20002478004	1
Cealo	Monoestearato de sorbitano	13209409	1
Euro OTC	Monoestearato de glicerol 60	16233804	1
Fagron	Monoestearato de glicerol...	12A27-N11	1
Fagron	Monoestearato de sorbitano	12E30-N14	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Monoestearato de glicerol…	12K05-N06	1
Fagron	Monoestearato de sorbitano	13B19-N01	1
Fagron	Monoestearato de sorbitano	13D10_N10	1
Fagron	Monoestearato de sorbitano	13D10-N10	1
Fagron	Monoestearato de sorbitano	14J07-B02-299399	1
Fagron	Monoestearato de glicerol 60	15009203	1
Fagron	Monoestearato de glicerol…	15280903	1
Fagron	Monoestearato de sorbitano	5052	1
Fagron	Monoestearato de glicerol…	7G19-N09	1
Fiebig	Monoestearato de glicerol…	20001564002	1
Gehe	Monoestearato de glicerol…	18328702	1
Gehe	Monoestearato de glicerol 60	19054702	1
Gehe	Monoestearato de glicerol…	20001564002	1
Ichthyol/Phoenix	Monoestearato de sorbitano	14372803	1
Krieger	Monoestearato de glicerol 60	19054702	1
L12	Monoestearato de glicerol 60	16233802	2
Nachprüfung	Monoestearato de sorbitano		1
Noweda	Monoestearato de glicerol…	11079301	1
Noweda	Monoestearato de glicerol 60	15009203	1
Noweda	Monoestearato de sorbitano	17178102	1
Noweda	Monoestearato de sorbitano	21001797001	1
Noweda	Monoestearato de sorbitano	22002437005	1
Phonix	Monoestearato de glicerol 60	13109304	1
Phonix	Monoestearato de sorbitano	13209418	1
Sanacorp	Monoestearato de sorbitano	22002437005	1
Spangropharm	Monoestearato de glicerol…	80402468	1

- 235 620 spectra from 1515 *Apo-Ident* customers from a total of 49 112 batches from a further 718 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Monoestearatos* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Monoestearatos* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	2050	0	150 912
Type B	0	1209	1	200 874
Type C	0	446	1	235 620

The substance/substance group *Monoestearatos* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.7073 %)
Type B	100.0000 % (> 99.9912 %)	99.9174 % (> 99.6694 %)
Type C	100.0000 % (> 99.9007 %)	99.7763 % (> 99.1051 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20691	21446	21,72	66,52
20751	20751	0,00	153,56
20783	20751	4,30	149,31
20828	22764	35,32	96,29
20867	21446	33,82	71,16
21093	21093	0,00	108,44
21437	21437	0,00	100,42
21446	21446	0,00	65,58
21545	21446	31,93	70,40
21576	21576	0,00	133,58
21585	21576	2,50	134,30
21885	21885	0,00	116,72
21982	22320	6,24	104,61
22277	25620	23,13	61,38
22320	22320	0,00	103,67
22464	22464	0,00	73,06
22623	22623	0,00	128,58
22667	20751	18,95	169,11
22764	22764	0,00	96,43
23188	23188	0,00	91,19
23706	22764	6,44	98,37
23831	23831	0,00	111,23
24025	24025	0,00	122,34
24371	24371	0,00	120,74
24673	24673	0,00	123,56
25094	25094	0,00	101,21
25385	22320	30,72	125,33
25564	25564	0,00	102,87
25618	25618	0,00	120,96
25620	25620	0,00	61,12
26004	26004	0,00	107,12
26018	26018	0,00	73,42
26235	25618	20,73	127,88
26369	26369	0,00	111,01
26480	26480	0,00	122,53
26728	26728	0,00	101,67
26729	26729	0,00	61,87
26958	26958	0,00	123,84

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
27257	27257	0,00	112,29
27316	27316	0,00	114,43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mupirocina cálcica**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20781-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mupirocina cálcica; Mupirocinum calcicum

Special notes

When selecting the *Mupirocina cálcica* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mupirocina cálcica	8	4	14

Second-stage model

For differentiation of the substance/substance group *Mupirocina cálcica* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mupirocina cálcica* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	85,18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mupirocina cálcica* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mupirocina cálcica*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mupirocina cálcica	14276602	21745	60	20141103
Caelo	Mupirocina cálcica	161184	22454	60	20160504*
Caelo	Mupirocina cálcica	18191606	25376	40	20180813
Caelo	Mupirocina cálcica	23003561	27116	40	20240202*
Caelo	Mupirocina cálcica	23003561	27116SI	20	20240202*
Fagron	Mupirocina cálcica	12E02-N07	20781	40	1401556
Fagron	Mupirocina cálcica	15H13-B01-316111	23213	40	20150909
Fagron	Mupirocina cálcica	18A16-B02-349169	25373	40	20180226
Fagron	Mupirocina cálcica	21K17-B01-219626	26152	40	20220426
Fagron	Mupirocina cálcica	21K17-B01-219626	26152SI	20	20220426

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Mupirocina cálcica*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 5 reference samples from the substance/substance group *Mupirocina cálcica*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mupirocina cálcica	161608	23860	40
Caelo	Mupirocina cálcica	21003209003	25856	50
Caelo	Mupirocina cálcica	22001500	26259	40
Euro OTC	Mupirocina cálcica	2001029	25297	40
Caelo	Mupirocina cálcica	22001500	26259SI	20

- 201 894 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 14 spectra from 11 *Apo-Ident* customers from 14 batches from the substance/substance group *Mupirocina cálcica*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Mupirocina cálcica	17356502	1
Caelo	Mupirocina cálcica	17356506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mupirocina cálcica	17356509	1
Caelo	Mupirocina cálcica	17F21-B03-34519	1
Caelo	Mupirocina cálcica	18191601	1
Caelo	Mupirocina cálcica	24041801	1
Caelo	Mupirocina cálcica	83200301013	1
Caelo	Mupirocina cálcica	9041801	1
Fagron	Mupirocina cálcica	14B03-B30-297291	1
Fagron	Mupirocina cálcica	15H13-B01	1
Fagron	Mupirocina cálcica	17F21-B03	1
Fagron	Mupirocina cálcica	17F21-B03-338597	1
Fagron	Mupirocina cálcica	17F21-B03-339080	1
Fagron	Mupirocina cálcica	83200340116	1

- 236 053 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mupirocina cálcica* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mupirocina cálcica* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	190	0	201 894
Type C	0	14	0	236 053

The substance/substance group *Mupirocina cálcica* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20781	20781	0,00	102,63
21745	22454	14,30	102,69
22454	22454	0,00	103,62
23213	27116	13,65	104,69
25373	27116	36,88	105,83
25376	27116	9,75	104,19
26152	27116	16,93	105,45
27116	27116	0,00	104,38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Naproxeno**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22316-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naproxeno; Naproxenum

Special notes

When selecting the *Naproxeno* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Naproxeno	5	2	3

Second-stage model

For differentiation of the substance/substance group *Naproxeno* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Naproxeno* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	99,84	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Naproxeno* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Naproxeno*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Naproxeno	15F18-B03-309492	22316	45	AR-16-FG-008486-02
Fagron	Naproxeno	15F18-B03-315691	22327	45	20150703
Fagron	Naproxeno	16B04-B09-326261	23105	40	20160229
Fagron	Naproxeno	22H17-B03-227263	26542	40	20221004
Fagron	Naproxeno	22H17-B03-227263	26542SI	20	20221004
Fagron	Naproxeno	23F19-B01-236106	27188	40	20230711
Fagron	Naproxeno	23F19-B01-236106	27188SI	20	20230711

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 250 spectra of 7 reference samples from the substance/substance group *Naproxeno*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 712 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Naproxeno*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Naproxeno	17C10-B03-336472	23763	40
Fagron	Naproxeno	21F15-B16-213613	25909	40
Fagron	Naproxeno	21F15-B16-213613	25909SI	10

- 201 994 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Naproxeno*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Naproxeno	13E31-B40-287536	2
Fagron	Naproxeno	16B04-B09-321569	24
Fagron	Naproxeno	17C10-B03-336472	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Naproxeno* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naproxeno* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	250	0	152 712
Type B	0	90	0	201 994
Type C	0	27	0	236 040

The substance/substance group *Naproxeno* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22316	22316	0,00	156,02
22327	22316	2,02	156,56
23105	22316	5,59	158,79
26542	22316	7,35	156,24
27188	22316	7,61	159,21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nicotinamida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20335-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nicotinamida; Nicotinamidum

Special notes

When selecting the *Nicotinamida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nicotinamida	9	13	54

Second-stage model

For differentiation of the substance/substance group *Nicotinamida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nicotinamida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	104,37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nicotinamida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nicotinamida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Nicotinamida	13097506	21364	40	20130416
Caelo	Nicotinamida	163048	23038	40	20161123*
Caelo	Nicotinamida	163048	23050	40	20161123*
Euro OTC	Nicotinamida	1310025-01	21643	60	20131121
Euro OTC	Nicotinamida	1511010	22251	60	20151203*
Euro OTC	Nicotinamida	1601045	22374	60	20160210*
Euro OTC	Nicotinamida	1610019	22874	40	20161202*
Euro OTC	Nicotinamida	1906027	24799	40	20190712*
Euro OTC	Nicotinamida	2009043	25407	40	20201012*
Euro OTC	Nicotinamida	2203037	26096	40	20220428*
Euro OTC	Nicotinamida	2203037	26096SI	20	20220428*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Nicotinamida*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 482 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 640 spectra of 16 reference samples from the substance/substance group *Nicotinamida*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Nicotinamida	11001809	20647	40
Caelo	Nicotinamida	161136	22434	60
Caelo	Nicotinamida	173419	23785	40
Caelo	Nicotinamida	190842	24525	40
Caelo	Nicotinamida	21003053	25861	50
Caelo	Nicotinamida	23002220	26960	40
Euro OTC	Nicotinamida	1707001	23555	40
Euro OTC	Nicotinamida	1801039	23957	40
Euro OTC	Nicotinamida	1812019	24493	40
Euro OTC	Nicotinamida	2001008	25071	40
Euro OTC	Nicotinamida	2105019	25704	50
Euro OTC	Nicotinamida	2309010	26931	40
Fagron	Nicotinamida	23A09-B01-226166	26906	40
Caelo	Nicotinamida	161136	22625	40
Euro OTC	Nicotinamida	2309010	26931SI	20
Fagron	Nicotinamida	23A09-B01-226166	26906SI	20

- 201 444 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 147 spectra from 81 *Apo-Ident* customers from 58 batches from the substance/substance group *Nicotinamida*.

- Among them are spectra of independent samples from 55 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nicotinamida	op12106006	1
AHD	Nicotinamida	2203037-03	1
Caelo	Nicotinamida	12133403	1
Caelo	Nicotinamida	12268302	1
Caelo	Nicotinamida	13097504	1
Caelo	Nicotinamida	13097506	1
Caelo	Nicotinamida	13352002	1
Caelo	Nicotinamida	14246806	1
Caelo	Nicotinamida	1511010-01	1
Caelo	Nicotinamida	1610019-01	1
Caelo	Nicotinamida	16113610	1
Caelo	Nicotinamida	16304803	1
Caelo	Nicotinamida	1707001-01	2
Caelo	Nicotinamida	17104108	2
Caelo	Nicotinamida	17341907	1
Caelo	Nicotinamida	1801039-01	1
Caelo	Nicotinamida	18214803	2
Caelo	Nicotinamida	20004516002	1
Caelo	Nicotinamida	2009043-01	1
Caelo	Nicotinamida	21000112003	2
Caelo	Nicotinamida	21000112006	1
Caelo	Nicotinamida	OP117072026	1
Caesar & Loretz GmbH	Nicotinamida	20004516002	1
DSM Nutritional Prod...	Nicotinamida	1106044-01	1
EuRho/Sanacorp	Nicotinamida	2001008-02	1
EuRho/Sanacorp	Nicotinamida	2009043-01	1
EuRho	Nicotinamida	200100801	1
EuRho	Nicotinamida	2203037-03	1
Euro OTC	Nicotinamida		1
Euro OTC	Nicotinamida	1108021-01	1
Euro OTC	Nicotinamida	11208021	1
Euro OTC	Nicotinamida	11401052	1
Euro OTC	Nicotinamida	1211031-02	5
Euro OTC	Nicotinamida	131002501	1
Euro OTC	Nicotinamida	1310025-01	4
Euro OTC	Nicotinamida	1408019-01	2
Euro OTC	Nicotinamida	1408019-19	1
Euro OTC	Nicotinamida	1503024-02	1
Euro OTC	Nicotinamida	1511010-01	5
Euro OTC	Nicotinamida	160104501	1
Euro OTC	Nicotinamida	1601045-01	5
Euro OTC	Nicotinamida	1610019-01	8
Euro OTC	Nicotinamida	1707001-01	12
Euro OTC	Nicotinamida	1801038-01	1
Euro OTC	Nicotinamida	1801039-01	10
Euro OTC	Nicotinamida	1906027-01	7
Euro OTC	Nicotinamida	1906027-01	1
Euro OTC	Nicotinamida	2001008-01	3
Euro OTC	Nicotinamida	2001008-02	4
Euro OTC	Nicotinamida	200904301	1
Euro OTC	Nicotinamida	2009043-01	7
Euro OTC	Nicotinamida	2009043-02	3
Euro OTC	Nicotinamida	2105019-01	1
Euro OTC	Nicotinamida	2203037-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nicotinamida	2203037-02	3
Euro OTC	Nicotinamida	2203037-03	1
Euro OTC	Nicotinamida	2610019-01	1
Euro OTC	Nicotinamida	OP11708013	2
Fagron	Nicotinamida	12J02-B03	1
Fagron	Nicotinamida	1801039-01	1
Fagron	Nicotinamida	20D06-F05-369981	1
Fagron	Nicotinamida	20F03-F04-371807	2
Fagron	Nicotinamida	21A14-F02	1
Fagron	Nicotinamida	L14020084	1
Gatt-Koller	Nicotinamida	221406112411	1
Gatt-Koller	Nicotinamida	4456/10104110	1
Gehe	Nicotinamida	2001008-02	1
Noweda	Nicotinamida	12133403	2
Noweda	Nicotinamida	22002418006	1
Phoenix	Nicotinamida	1211031-02	1
Phoenix	Nicotinamida	2001008-01	1
Sanacorp	Nicotinamida	2009043-01	1
Sanacorp	Nicotinamida	22002418003	1
sanacorp	Nicotinamida	oP12106006	1
VDL;16.04.15;5,60EUR	Nicotinamida	1408019-01	1

- 235 920 spectra from 1515 *Apo-Ident* customers from a total of 49 203 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nicotinamida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nicotinamida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	640	0	201 444
Type C	0	147	0	235 920

The substance/substance group *Nicotinamida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0625 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.9184 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21364	22251	7,02	276,46
21643	22251	4,32	276,07
22251	22251	0,00	275,65
22374	22374	0,00	274,28
22874	22874	0,00	273,86
23038	23038	0,00	274,93
23050	23050	0,00	275,03
24799	24799	0,00	276,62
25407	25407	0,00	278,11
26096	26096	0,00	277,58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nifedipina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10003587-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nifedipina; Nifedipinum

Special notes

When selecting the *Nifedipina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nifedipina	3	1	2

Second-stage model

For differentiation of the substance/substance group *Nifedipina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nifedipina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citrato de cafeína	168,63	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nifedipina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nifedipina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Nifedipina	21B18-F02-378364	26067	40	20210609
Fagron	Nifedipina	22G07-B03-218877	26469	40	230502385
Fagron	Nifedipina	22G07-B03-218877	26469SI	20	230502385
Fagron	Nifedipina	23F29-B05-228724	26900	40	20220803
Fagron	Nifedipina	23F29-B05-228724	26900SI	20	20220803

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 5 reference samples from the substance/substance group *Nifedipina*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 802 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Nifedipina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Nifedipina	18K19-B02-363428	25056	40
Fagron	Nifedipina	21B18-F02-378364	26067SI†	20

- 202 024 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Nifedipina*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nifedipina	21829-25-4	1
	Nifedipina	22G07-B03-218877	1
Sanacorp	Nifedipina	22G07-B03	1

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nifedipina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nifedipina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	60	0	202 024
Type C	0	3	0	236 064

The substance/substance group *Nifedipina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26067	26469	32,07	348,10
26469	26469	0,00	350,65
26900	26469	9,86	351,74

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nistatina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20116-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nistatina

Special notes

When selecting the *Nistatina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nistatina	12	7	247

Second-stage model

For differentiation of the substance/substance group *Nistatina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nistatina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	54,36	28,25
⋮	⋮	⋮
Bacitracina	>50	15,86
Anfotericina B	>50	21,64
Vitamina E acetato pó 50%	>50	33,00
Sulfato de colistina	>50	35,81
Cianocobalamina	>50	36,74
Levedura de selênio	>50	41,82
Riboflavina	>50	51,39
Glicerofosfato de cálcio	>50	56,20
Estradiol hemi-hidratado	>50	63,12
Estriol	>50	76,76
Triancinolona	>50	87,61
Pantotenato de cálcio	>50	93,94
Carmelose sódica	>50	99,72
SyrSpend® SF pH4 neo	>50	112,33
Gelatina, branca	>50	121,88
SyrSpend® SF Alka	>50	133,13
Metilcobalamina	>50	146,52
Bromidrato de hioscina	>50	151,37
Tosilcloramida sódica	>50	153,08
Amido de arroz	>50	170,86
Amido de milho	>50	213,76
Ácido oxálico	>50	240,40
SyrSpend® SF pH4	>50	288,89
Goma arábica, dispersão seca	>50	320,04
Amido de trigo	>50	331,42
Maltodextrina	>50	335,81
Fécula de batata	>50	354,51
Frutose	>50	518,85

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nistatina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nistatina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Nistatina	AP4018717N	23985	40	20160307
Caelo	Nistatina	16272214	23711	40	20160929
Caelo	Nistatina	17025110	23984	40	20170308
Caelo	Nistatina	21004088001	26305	30	20220201
Caelo	Nistatina	21004088001	26305SI	20	20220201
Euro OTC	Nistatina	1712010-01	24103	40	1807445
Euro OTC	Nistatina	1905014	24780	40	20190709*
Euro OTC	Nistatina	2006026	25354	40	20200907*
Euro OTC	Nistatina	2111001	25879	50	20211210*
Euro OTC	Nistatina	2301016	26595	40	20230214*
Euro OTC	Nistatina	2301016	26595SI	20	20230214*
Fagron	Nistatina	19B28-B05-191210	24645	40	20190316
Fagron	Nistatina	19H08-B04-200385	25722	50	20190823
Fagron	Nistatina	22A18-B07-218934	26381	40	20220325
Fagron	Nistatina	22A18-B07-218934	26381SI	20	20220325

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 15 reference samples from the substance/substance group *Nistatina*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.
- 152 412 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 8 reference samples from the substance/substance group *Nistatina*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Nistatina	20000969005	25435	40
Caelo	Nistatina	23001392	26843	40
Caelo	Nistatina	24000661	27326	40
Euro OTC	Nistatina	1612001-03	23727	40
Euro OTC	Nistatina	2310010	27005	40
Fagron	Nistatina	16L21-B01-338864	23712	40
Fagron	Nistatina	22I27-B12-225522	26460	40
Euro OTC	Nistatina	2111001	25879SI[†]	10

- 201 794 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1880 spectra from 762 *Apo-Ident* customers from 253 batches from the substance/substance group *Nistatina*.
- Among them are spectra of independent samples from 245 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nistatina		1
	Nistatina	2006026-02	1
	Nistatina	21004088006	1
	Nistatina	211100-02	1
	Nistatina	2111001-03	4
	Nistatina	22002863006	2
	Nistatina	22002863011	6
	Nistatina	230000218004	1
	Nistatina	23000218004	10
	Nistatina	23000218005	2
	Nistatina	23000218006	20
	Nistatina	23001392005	1
	Nistatina	23001392006	1
	Nistatina	2301016-01	33
	Nistatina	2310010-01	9
	Nistatina	24000661004	2
	Nistatina	26001021A	1
	Nistatina	37401222	1
1712010-02	Nistatina	2164071	1
AHC	Nistatina	2301016-01	1
AHD/Euro	Nistatina	1712010-01	1
AHD	Nistatina	1612001-01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Nistatina	18072114	1
AHD	Nistatina	23000218005	1
AHD	Nistatina	23001392004	1
AHD	Nistatina	2301016-01	2
Alliance Healthcare	Nistatina	1905014-03	1
Alliance Healthcare	Nistatina	2006026-01	1
Alliance Healthcare	Nistatina	2006026-02	3
Alliance/EurRho	Nistatina	2006026-0231	1
Alliance	Nistatina	2111001-02	1
Alliance	Nistatina	2301016-01	1
Antibiotice S.A., RO	Nistatina	21000074004	2
Antibiotice SA Iasi/ AHD	Nistatina	1712010-01	1
Antibiotice/Noweda	Nistatina	4019851	3
Antibiotice	Nistatina	1712010-01	2
Anzag	Nistatina	1712010-01	1
Anzag	Nistatina	2310010-01	1
Anzag	Nistatina	2902041-02	1
Apo Ident	Nistatina	2006026-01	1
Apo Ident	Nistatina	800219	1
ApoHo 20.6.17	Nistatina	1722	1
apo-ident/Alliance	Nistatina	2006026-01	1
apo-ident/Phoenix	Nistatina	191220111	1
Apo-ident	Nistatina	1905014-02	1
Apo-ident	Nistatina	2006026-02	2
apomix	Nistatina	2006026-01	1
apomix	Nistatina	2111001-02	1
apotec / AHD	Nistatina	1905014-01	1
apotec	Nistatina	1905014-01	1
Bombastus	Nistatina	1212024-01	1
Caelo	Nistatina	1(18072128)	1
Caelo	Nistatina	11069704	1
Caelo	Nistatina	11069706	2
Caelo	Nistatina	11069716	1
Caelo	Nistatina	11069719	1
Caelo	Nistatina	11069730	1
Caelo	Nistatina	11069731	1
Caelo	Nistatina	1107046-01	1
Caelo	Nistatina	11071894	1
Caelo	Nistatina	12017003	1
Caelo	Nistatina	12017004	4
Caelo	Nistatina	12017009	1
Caelo	Nistatina	12017010	1
Caelo	Nistatina	12017011	2
Caelo	Nistatina	12017015	2
Caelo	Nistatina	12138021	2
Caelo	Nistatina	12158004	3
Caelo	Nistatina	12158005	1
Caelo	Nistatina	12158006	7
Caelo	Nistatina	12158008	3
Caelo	Nistatina	12158009	1
Caelo	Nistatina	12158010	4
Caelo	Nistatina	12158019	3
Caelo	Nistatina	12158020	1
Caelo	Nistatina	12158021	2
Caelo	Nistatina	12158022	1
Caelo	Nistatina	121580921	1
Caelo	Nistatina	12158oo4	1
Caelo	Nistatina	13101201	1
Caelo	Nistatina	13101202	1
Caelo	Nistatina	13173401	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nistatina	13173408	1
Caelo	Nistatina	14363514	1
Caelo	Nistatina	15335310	1
Caelo	Nistatina	1612001	1
Caelo	Nistatina	1612001-03	1
Caelo	Nistatina	16272203	2
Caelo	Nistatina	16L21-B01-338876	1
Caelo	Nistatina	1712010-01	8
Caelo	Nistatina	17400520	1
Caelo	Nistatina	18072014	1
Caelo	Nistatina	18072104	2
Caelo	Nistatina	18072105	6
Caelo	Nistatina	18072107	1
Caelo	Nistatina	18072108	8
Caelo	Nistatina	18072109	11
Caelo	Nistatina	18072112	4
Caelo	Nistatina	18072113	28
Caelo	Nistatina	18072114	18
Caelo	Nistatina	18072118	2
Caelo	Nistatina	18072120	9
Caelo	Nistatina	18072121	8
Caelo	Nistatina	18072123	17
Caelo	Nistatina	18072124	13
Caelo	Nistatina	18072126	2
Caelo	Nistatina	18072128	5
Caelo	Nistatina	18072128P-190709-1	1
Caelo	Nistatina	18072129	4
Caelo	Nistatina	1807213	2
Caelo	Nistatina	183034004	1
Caelo	Nistatina	19026806	1
Caelo	Nistatina	19028801	27
Caelo	Nistatina	19028803	2
Caelo	Nistatina	19028805	1
Caelo	Nistatina	19028806	19
Caelo	Nistatina	19028808	14
Caelo	Nistatina	19028809	27
Caelo	Nistatina	1902881	1
Caelo	Nistatina	19028810	1
Caelo	Nistatina	19028811	1
Caelo	Nistatina	19028813	16
Caelo	Nistatina	1903034005	1
Caelo	Nistatina	19034004	1
Caelo	Nistatina	1905014-01	3
Caelo	Nistatina	1905014-02	1
Caelo	Nistatina	19058809	1
Caelo	Nistatina	19303034009	1
Caelo	Nistatina	193034003	15
Caelo	Nistatina	193034004	21
Caelo	Nistatina	193034005	3
Caelo	Nistatina	193034009	14
Caelo	Nistatina	19304004	1
Caelo	Nistatina	19B28-B06-196732	1
Caelo	Nistatina	20000096006	1
Caelo	Nistatina	2000096006	1
Caelo	Nistatina	20000969002	3
Caelo	Nistatina	20000969005	24
Caelo	Nistatina	20000969006	12
Caelo	Nistatina	2000096902	1
Caelo	Nistatina	20002487001	1
Caelo	Nistatina	20002487004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nistatina	20004452001	3
Caelo	Nistatina	20004452002	15
Caelo	Nistatina	20004452003	22
Caelo	Nistatina	2000969005	1
Caelo	Nistatina	2006026-02	2
Caelo	Nistatina	2091304	1
Caelo	Nistatina	210000740004	1
Caelo	Nistatina	21000074001	1
Caelo	Nistatina	21000074003	2
Caelo	Nistatina	21000074004	30
Caelo	Nistatina	21000074005	23
Caelo	Nistatina	21000074008	1
Caelo	Nistatina	2100074004	1
Caelo	Nistatina	2100074005	1
Caelo	Nistatina	210021650009	1
Caelo	Nistatina	21002165001	14
Caelo	Nistatina	21002165002	4
Caelo	Nistatina	21002165003	14
Caelo	Nistatina	21002165006	1
Caelo	Nistatina	21002165007	14
Caelo	Nistatina	21002165009	10
Caelo	Nistatina	21004088001	13
Caelo	Nistatina	21004088004	2
Caelo	Nistatina	21004088006	7
Caelo	Nistatina	21004088008	3
Caelo	Nistatina	2111001-03	1
Caelo	Nistatina	22002863002	1
Caelo	Nistatina	22002863006	1
Caelo	Nistatina	22002863010	1
Caelo	Nistatina	22002863011	2
Caelo	Nistatina	23000218006	1
Caelo	Nistatina	3101201	1
Caelo	Nistatina	3338	1
Caelo	Nistatina	4010914	1
Caelo	Nistatina	485870081652	1
Caelo	Nistatina	6082013B	1
Caelo	Nistatina	81072113	1
Caelo	Nistatina	930340031	1
Caelo	Nistatina	C129330	1
Caesar & Loretz GmbH...	Nistatina	18072124	1
Caesar & Loretz GmbH...	Nistatina	1712010-01	1
Caesar & Loretz GmbH...	Nistatina	19028810	1
Caesar & Loretz GmbH...	Nistatina	21004088006	1
Caesar & Loretz GmbH...	Nistatina	18072128	1
Caesar & Loretz GmbH...	Nistatina	19028809	1
Caesar & Loretz GmbH...	Nistatina	19028809	1
Caesar & Loretz GmbH...	Nistatina	21000074005	1
Caesar & Loretz GmbH...	Nistatina	19028813	1
Caesar & Loretz GmbH...	Nistatina	21000074004	1
Caesar & Loretz GmbH...	Nistatina	22002863011	1
Caesar & Loretz GmbH/AEP	Nistatina	23000218004	1
Caesar & Loretz GmbH...	Nistatina	19028809	1
Caesar & Loretz GmbH...	Nistatina	20000969005	2
Caesar & Loretz GmbH...	Nistatina	21000074004	1
Caesar & Loretz GmbH...	Nistatina	20004452003	1
Caesar & Loretz GmbH/Gehe	Nistatina	193034004	2
Caesar & Loretz GmbH/Gehe	Nistatina	20000969005	2
Caesar & Loretz GmbH/Gehe	Nistatina	20004452002	1
Caesar & Loretz GmbH...	Nistatina	20004452001	1
Caesar & Loretz GmbH...	Nistatina	19028808	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Nistatina	21002165001	1
Caesar & Loretz GmbH...	Nistatina	21002165001	1
Caesar & Loretz GmbH...	Nistatina	193034009	1
Caesar & Loretz GmbH...	Nistatina	21000074004	1
Caesar & Loretz GmbH/K	Nistatina	19028810	1
Caesar & Loretz GmbH/K	Nistatina	21004088001	1
Caesar & Loretz GmbH/kehr	Nistatina	19028813	1
Caesar & Loretz GmbH...	Nistatina	19028813	3
Caesar & Loretz GmbH...	Nistatina	193034009	2
Caesar & Loretz GmbH...	Nistatina	19028808	1
Caesar & Loretz GmbH...	Nistatina	193034009	1
Caesar & Loretz GmbH...	Nistatina	2006026-01	1
Caesar & Loretz GmbH...	Nistatina	21002165003	2
Caesar & Loretz GmbH...	Nistatina	21002165009	1
Caesar & Loretz GmbH...	Nistatina	20000969005	1
Caesar & Loretz GmbH...	Nistatina	21004088001	1
Caesar & Loretz GmbH...	Nistatina	21004088006	1
Caesar & Loretz GmbH...	Nistatina	20000969006	1
Caesar & Loretz GmbH...	Nistatina	210000745005	1
Caesar & Loretz GmbH...	Nistatina	21004088001	1
Caesar & Loretz GmbH/Sa	Nistatina	19028806	1
Caesar & Loretz GmbH...	Nistatina	19028801	1
Caesar & Loretz GmbH...	Nistatina	193034003	1
Caesar & Loretz GmbH...	Nistatina	193034004	1
Caesar & Loretz GmbH...	Nistatina	20000969006	1
Caesar & Loretz GmbH...	Nistatina	20004452002	1
Caesar & Loretz GmbH...	Nistatina	20004452003	1
Caesar & Loretz GmbH...	Nistatina	21000074005	1
Caesar & Loretz GmbH...	Nistatina	21004088008	1
Caesar & Loretz GmbH	Nistatina	18072113	3
Caesar & Loretz GmbH	Nistatina	18072120	1
Caesar & Loretz GmbH	Nistatina	18072123	5
Caesar & Loretz GmbH	Nistatina	18072124	3
Caesar & Loretz GmbH	Nistatina	18072128	3
Caesar & Loretz GmbH	Nistatina	18072129	3
Caesar & Loretz GmbH	Nistatina	19028801	9
Caesar & Loretz GmbH	Nistatina	19028806	3
Caesar & Loretz GmbH	Nistatina	19028808	8
Caesar & Loretz GmbH	Nistatina	19028809	5
Caesar & Loretz GmbH	Nistatina	19028813	5
Caesar & Loretz GmbH	Nistatina	193034003	7
Caesar & Loretz GmbH	Nistatina	193034004	6
Caesar & Loretz GmbH	Nistatina	193034005	4
Caesar & Loretz GmbH	Nistatina	193034009	6
Caesar & Loretz GmbH	Nistatina	20000969002	1
Caesar & Loretz GmbH	Nistatina	20000969005	7
Caesar & Loretz GmbH	Nistatina	20000969006	11
Caesar & Loretz GmbH	Nistatina	20004452001	3
Caesar & Loretz GmbH	Nistatina	20004452002	13
Caesar & Loretz GmbH	Nistatina	20004452003	4
Caesar & Loretz GmbH	Nistatina	2000969006	2
Caesar & Loretz GmbH	Nistatina	21000074003	5
Caesar & Loretz GmbH	Nistatina	21000074004	6
Caesar & Loretz GmbH	Nistatina	21000074005	7
Caesar & Loretz GmbH	Nistatina	21000074008	1
Caesar & Loretz GmbH	Nistatina	21002165001	6
Caesar & Loretz GmbH	Nistatina	21002165002	2
Caesar & Loretz GmbH	Nistatina	21002165007	7
Caesar & Loretz GmbH	Nistatina	21002165009	3
Caesar & Loretz GmbH	Nistatina	21004088001	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Nistatina	21004088004	1
Caesar & Loretz GmbH	Nistatina	21004088006	1
Caesar & Loretz GmbH	Nistatina	21004088008	2
Caesar & Loretz GmbH	Nistatina	22002863006	2
Caesar & Loretz GmbH	Nistatina	23000218004	1
Caesar & Loretz Hilden	Nistatina	18072112	2
Caesar & Loretz Hilden	Nistatina	18293404	1
Caesar & Loretz Hilden	Nistatina	19028801	1
Caesar & Loretz/Geil...	Nistatina	19028806	1
Caesar & Loretz/Geil...	Nistatina	19028809	2
Caesar & Loretz/Noweda	Nistatina	193034004	2
Caesar & Loretz/Phoenix	Nistatina	20004452002	1
Caesar&Lorenz / Gehe	Nistatina	19028810	1
Caesar&Lorenz	Nistatina	2100074004	1
Caesar&Lorenz	Nistatina	21002165001	1
Caesar&Lorenz	Nistatina	21002165007	1
Caesar&loretz,Anzag	Nistatina	12158008	3
Caesar&loretz,Phoenix	Nistatina	1218008	1
Caesar&loretz,Phoenix	Nistatina	13173401	4
Caesar&loretz,Phoenix	Nistatina	13173408	1
Caesar&loretz,Phoenix	Nistatina	14196509	2
Caesar&loretz,Phoenix	Nistatina	14363512	1
caewlo	Nistatina	21004088001	1
Canea Pharma GmbH	Nistatina	18072121	1
Cealo/ AHD	Nistatina	19028801	1
Cealo/Alliance Healthcare	Nistatina	18072118	1
DSM Caüua S.p.A	Nistatina	1207009-01	1
Eu Rho Pharm/ K	Nistatina	2006026-01	1
Eurho Phönix	Nistatina	2006026	1
Eurho Phönix	Nistatina	2111001-02	3
EuRho/Anzag	Nistatina	1107036-01	1
EuRho/Anzag	Nistatina	1712010-02	1
EuRho/Fiebig	Nistatina	1905014-01	4
Eurho/Fiebig	Nistatina	8000219	1
EuRho/Noweda	Nistatina	2006026-02	1
EuRho/Noweda	Nistatina	2111001-02	1
EuRho/Phoenix	Nistatina	1712010-01	2
EuRho/Sanacorp	Nistatina	1712010-02	2
EuRho/Sanacorp	Nistatina	2006026-02	1
Eurho/Synoph	Nistatina	200602-03	4
Eurho/Synoph	Nistatina	2006026-02	1
EuRho	Nistatina	1107046-01	1
EuRho	Nistatina	1207009-01	1
EuRho	Nistatina	1503021-02	2
EuRho	Nistatina	1712010-01	1
EuRho	Nistatina	1905014-02	2
EuRho	Nistatina	2006026-01	1
EuRho	Nistatina	2006026-02	1
EuRho	Nistatina	2111001-02	1
Euro Gehe	Nistatina	1712010-01	1
Euro Noweda	Nistatina	26001021A	1
Euro OTC	Nistatina	1107036-01	4
Euro OTC	Nistatina	1107046-01	2
Euro OTC	Nistatina	1111057-01	7
Euro OTC	Nistatina	1207009-01	7
Euro OTC	Nistatina	1207009-02	2
Euro OTC	Nistatina	121024-01	1
Euro OTC	Nistatina	1212024-01	14
Euro OTC	Nistatina	1212024-02	13
Euro OTC	Nistatina	127009-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nistatina	130705301	1
Euro OTC	Nistatina	1307053-01	5
Euro OTC	Nistatina	1307053-02	2
Euro OTC	Nistatina	1511020-01	1
Euro OTC	Nistatina	1511020-02	1
Euro OTC	Nistatina	16120001-02	1
Euro OTC	Nistatina	1612001-01	4
Euro OTC	Nistatina	1612001-02	1
Euro OTC	Nistatina	161200103	3
Euro OTC	Nistatina	1612001-03	8
Euro OTC	Nistatina	1712010	1
Euro OTC	Nistatina	171201001	1
Euro OTC	Nistatina	1712010-01	99
Euro OTC	Nistatina	171201002	4
Euro OTC	Nistatina	1712010-02	47
Euro OTC	Nistatina	1712010-12	1
Euro OTC	Nistatina	1712020-01	2
Euro OTC	Nistatina	17400520	6
Euro OTC	Nistatina	18072114	1
Euro OTC	Nistatina	18072124	2
Euro OTC	Nistatina	190501-01	1
Euro OTC	Nistatina	19050114-01	1
Euro OTC	Nistatina	1905014	2
Euro OTC	Nistatina	190501401	2
Euro OTC	Nistatina	1905014-01	120
Euro OTC	Nistatina	1905014-02	40
Euro OTC	Nistatina	1905014-03	11
Euro OTC	Nistatina	190514-02	1
Euro OTC	Nistatina	19500711	1
Euro OTC	Nistatina	20006026-01	1
Euro OTC	Nistatina	20006026-02	1
Euro OTC	Nistatina	2003026-01	1
Euro OTC	Nistatina	2006012501	1
Euro OTC	Nistatina	200602302	1
Euro OTC	Nistatina	2006023-02	1
Euro OTC	Nistatina	2006025-2	1
Euro OTC	Nistatina	2006026	1
Euro OTC	Nistatina	2006026-01	47
Euro OTC	Nistatina	200602602	1
Euro OTC	Nistatina	2006026-02	86
Euro OTC	Nistatina	2006026-026	1
Euro OTC	Nistatina	2006026-03	1
Euro OTC	Nistatina	2006026-23	1
Euro OTC	Nistatina	2006226-02	1
Euro OTC	Nistatina	200626-01	2
Euro OTC	Nistatina	200626-02	1
Euro OTC	Nistatina	21000074004	1
Euro OTC	Nistatina	2111001_03	1
Euro OTC	Nistatina	2111001-01	12
Euro OTC	Nistatina	2111001-02	46
Euro OTC	Nistatina	2111001-03	2
Euro OTC	Nistatina	2111011-02	1
Euro OTC	Nistatina	2301016-01	8
Euro OTC	Nistatina	26001021A	1
Euro OTC	Nistatina	2811032-01	1
Euro OTC	Nistatina	4014991	1
Euro OTC	Nistatina	4019851	3
Euro OTC	Nistatina	6026-01	1
Euro OTC	Nistatina	702270	1
Euro OTC	Nistatina	8000219	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nistatina	AP200923-01	1
Euro OTC	Nistatina	C129440	1
Euro OTC	Nistatina	C129531	2
Euro OTC	Nistatina	C129854	1
Euro OTC	Nistatina	Nys011222	1
EUro/AHD	Nistatina	1307053-01	1
Euro/Gehe	Nistatina	1905014-01	1
Euro/Gehe	Nistatina	2006026-01	1
Euro/Gehe	Nistatina	2006026-02	1
Euro/Jenne	Nistatina	2006026-02	1
Euro/Phoenix	Nistatina	1905014-03	1
Europharm/Otto	Nistatina	1107046-01	1
Fagron	Nistatina		1
Fagron	Nistatina	11000422a	1
Fagron	Nistatina	11C21-N10	1
Fagron	Nistatina	11K11-No4	1
Fagron	Nistatina	12C29-N09	1
Fagron	Nistatina	12G04-N12	1
Fagron	Nistatina	13C11-N08	1
Fagron	Nistatina	16L21-B01	1
Fagron	Nistatina	17B01-B11-338878	1
Fagron	Nistatina	17J25-B01-344221	1
Fagron	Nistatina	17J25-B01-348043	2
Fagron	Nistatina	18072112	1
Fagron	Nistatina	18900619B	1
Fagron	Nistatina	1905014-01	1
Fagron	Nistatina	19828	1
Fagron	Nistatina	19B28-B05-191208	2
Fagron	Nistatina	19B28-B05-191210	2
Fagron	Nistatina	19H08-B04-200385	2
Fagron	Nistatina	20121202	1
Fagron	Nistatina	20H18-B13-201282	1
Fagron	Nistatina	20H18B13201991	1
Fagron	Nistatina	20H18-B13-201991	2
Fagron	Nistatina	21H13-B01-214453	1
Fagron	Nistatina	4014376	1
Fagron	Nistatina	B01-2144503	1
Fagron	Nistatina	b04-2003805	1
Gatt-Koller	Nistatina	1900206	2
Gehe amax	Nistatina	1712010-01	1
Gehe amax	Nistatina	1905014-01	1
Gehe Rostock	Nistatina	2111001-02	1
Gehe/EuRho	Nistatina	1905014-02	1
Gehe	Nistatina	1107036-01	1
Gehe	Nistatina	1111057-01	1
Gehe	Nistatina	1207009-01	1
Gehe	Nistatina	12158008	1
Gehe	Nistatina	1307053-02	1
Gehe	Nistatina	1712010-01	1
Gehe	Nistatina	1712010-02	1
Gehe	Nistatina	1905014-01	1
Gehe	Nistatina	1905014-03	1
Gehe	Nistatina	20000969005	3
Gehe	Nistatina	200602601	1
Gehe	Nistatina	21000074004	1
GEHE	Nistatina	22002863006	1
Gehe	Nistatina	2301016-01	1
GEHE	Nistatina	2301016-01	1
Geilenkirchen	Nistatina	1905014-01	1
Jenne	Nistatina	21000074003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Nistatina	1612001-02	1
Kehr	Nistatina	18072123	1
Kehr	Nistatina	2301016-01	2
L12	Nistatina	1712010-01	1
Nachprüfung	Nistatina	1118E-01941	1
Nachprüfung	Nistatina	123456	1
Noweda Taucha	Nistatina	2111001-01	1
Noweda	Nistatina	1207009-01	1
Noweda	Nistatina	19028801	1
Noweda	Nistatina	19028808	1
Noweda	Nistatina	21000074005	2
Noweda	Nistatina	21002165001	2
Noweda	Nistatina	2111001-02	1
Noweda	Nistatina	22002863006	2
Noweda	Nistatina	22002863011	1
Noweda	Nistatina	23000218004	2
Noweda	Nistatina	23000218006	1
Noweda	Nistatina	23001392006	1
Noweda	Nistatina	2301016-01	2
Nystatin	Nistatina	1905014-01	1
Otto Geilenkirchen	Nistatina	22002863011	1
Otto Geilenkirchen	Nistatina	2300218004	1
ph.Eur	Nistatina	2111001-02	1
Phoenix/apotec	Nistatina	2301016-01	1
Phoenix	Nistatina	1712010-01	1
Phoenix	Nistatina	1712010-02	1
Phoenix	Nistatina	17400520	1
Phoenix	Nistatina	1905014-01	2
Phoenix	Nistatina	20004452003	1
Phoenix	Nistatina	21002165003	1
Phoenix	Nistatina	23000218005	1
Phoenix	Nistatina	23000218006	1
Phoenix	Nistatina	3361	1
Phoenix	Nistatina	3410	1
Phönix Gotha	Nistatina	1712010-02	1
Phönix/Euro	Nistatina	1111057-01	1
Phönix	Nistatina	12017005	2
Phönix	Nistatina	1212024-01	1
Phönix	Nistatina	1212024-02	1
Phönix	Nistatina	12158010	1
Phönix	Nistatina	1712010-01	1
Phönix	Nistatina	18072109	1
Phönix	Nistatina	18072121	1
Phönix	Nistatina	19028813	1
Phönix	Nistatina	1905014-01	4
Phönix	Nistatina	1905014-02	1
Phönix	Nistatina	1930343004	1
Phönix	Nistatina	20000969005	1
Phönix	Nistatina	2006026-01	1
Phönix	Nistatina	2006026-02	2
Phönix	Nistatina	2111001-01	1
Phönix	Nistatina	23000218006	5
Phönix	Nistatina	2301016-01	1
Phönix	Nistatina	37401222	1
Sanacorp/Caesar & Lo…	Nistatina	18072120	1
Sanacorp/EuRho	Nistatina	171201001	1
Sanacorp	Nistatina	1107046-01	1
Sanacorp	Nistatina	1212024-02	1
sanacorp	Nistatina	19028808	1
Sanacorp	Nistatina	193034009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Nistatina	20004452002	1
Sanacorp	Nistatina	2002863011	1
Sanacorp	Nistatina	21002165003	1
Sanacorp	Nistatina	21004088006	1
Sanacorp	Nistatina	23000218006	2
Sanacorp	Nistatina	23001392006	1
Sanacorp	Nistatina	2301016-01	4
Sanacorp	Nistatina	24000661003	1
Sanacorp	Nistatina	24000661004	1
VUAB Pharma / Gehe	Nistatina	2006026-02	1
VUAB Pharma	Nistatina	17400520	2
VUAB Pharma	Nistatina	2111001-02	1
VUAB/Noweda	Nistatina	8000219	1

- 234 187 spectra from 1515 *Apo-Ident* customers from a total of 49 012 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nistatina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nistatina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	550	0	152 412
Type B	0	290	0	201 794
Type C	0	1760	120	234 187

The substance/substance group *Nistatina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9091 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9007 %)	93.6170 % (> 93.4574 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23711	24780	16,83	95,20
23984	26595	19,47	102,63
23985	26595	19,20	105,57
24103	24103	0,00	100,52
24645	24780	16,84	102,75
24780	24780	0,00	103,28
25354	25354	0,00	87,75
25722	24780	26,72	93,13
25879	25879	0,00	79,41
26305	26595	24,87	96,92
26381	24780	8,23	100,45
26595	26595	0,00	106,14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nitrato de miconazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20210-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nitrato de miconazol; Miconazol, nitrato; Miconazoli nitras

Special notes

When selecting the *Nitrato de miconazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nitrato de miconazol	7	16	477

Second-stage model

For differentiation of the substance/substance group *Nitrato de miconazol* the following second-stage model is used:

- Submodelo 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nitrato de miconazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	148,51	–
⋮	⋮	⋮
Mesalazina	>50	65,94
Clioquinol	>50	118,15
Ácido nicotínico	>50	160,79
Teofilina etilenodiamina hidratada	>50	253,84

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nitrato de miconazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nitrato de miconazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Nitrato de miconazol	13185601	20875	40	20130704
Caelo	Nitrato de miconazol	13185601	20905	80	20130704
Caelo	Nitrato de miconazol	13352802	21350	39	1412250
Caelo	Nitrato de miconazol	13352802	21351	40	20131118
Caelo	Nitrato de miconazol	161447	22630	40	20160617*
Euro OTC	Nitrato de miconazol	1307025-02	21649	60	20130806
Euro OTC	Nitrato de miconazol	1509014	21900	60	20150930*
Fagron	Nitrato de miconazol	13D22-N14	20817	100	20130529
Fagron	Nitrato de miconazol	18C23-B02-356141	24593	40	20180416

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 499 spectra of 9 reference samples from the substance/substance group *Nitrato de miconazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 463 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 670 spectra of 18 reference samples from the substance/substance group *Nitrato de miconazol*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Nitrato de miconazol	172175	23662	30
Caelo	Nitrato de miconazol	182821	24388	40
Caelo	Nitrato de miconazol	21000827011	26621	40
Euro OTC	Nitrato de miconazol	1604004	22522	40
Euro OTC	Nitrato de miconazol	1607004	22671	40
Euro OTC	Nitrato de miconazol	1611024	22920	40
Euro OTC	Nitrato de miconazol	1705039	23429	40
Euro OTC	Nitrato de miconazol	1710020	23775	40
Euro OTC	Nitrato de miconazol	1803028	24071	40
Euro OTC	Nitrato de miconazol	1811015	24338	40
Euro OTC	Nitrato de miconazol	1904032	24601	40
Euro OTC	Nitrato de miconazol	1909029	24938	40
Euro OTC	Nitrato de miconazol	2009034	25417	40
Euro OTC	Nitrato de miconazol	2103012	25676	40
Euro OTC	Nitrato de miconazol	2210002	26427	40
Fagron	Nitrato de miconazol	22F08-B02-221067	26173	40
Caelo	Nitrato de miconazol	21000827011	26621SI	20
Fagron	Nitrato de miconazol	22F08-B02-221067	26173SI	20

- 201 414 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3256 spectra from 843 *Apo-Ident* customers from 510 batches from the substance/substance group *Nitrato de miconazol*.
- Among them are spectra of independent samples from 475 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nitrato de miconazol	2009034-02	1
	Nitrato de miconazol	210008270022	1
	Nitrato de miconazol	21000827013	1
	Nitrato de miconazol	21000827016	4
	Nitrato de miconazol	21000827017	2
	Nitrato de miconazol	21000827018	2
	Nitrato de miconazol	21000827019	1
	Nitrato de miconazol	21000827021	1
	Nitrato de miconazol	21000827022	3
	Nitrato de miconazol	21000827023	7
	Nitrato de miconazol	21000827024	4
	Nitrato de miconazol	21000827025	9
	Nitrato de miconazol	21000827026	10
	Nitrato de miconazol	2100087024	1
	Nitrato de miconazol	2103012-02	1
	Nitrato de miconazol	2210002	1
	Nitrato de miconazol	2210002-0	1
	Nitrato de miconazol	2210002-01	10
	Nitrato de miconazol	22832-87-7	1
	Nitrato de miconazol	22F08-B02-213149	1
	Nitrato de miconazol	22F08-B02-213580	1
	Nitrato de miconazol	22F08-B02-221067	3
	Nitrato de miconazol	23000589001	3
	Nitrato de miconazol	23000589003	3
	Nitrato de miconazol	23000589004	8
	Nitrato de miconazol	23003273002	1
	Nitrato de miconazol	23003273006	1
	Nitrato de miconazol	2300589001	1
	Nitrato de miconazol	2311020-01	2
	Nitrato de miconazol	B02-221067	1
	Nitrato de miconazol	B09-2402706	1
18282105	Nitrato de miconazol	8704870	1
18282114	Nitrato de miconazol	CAELO	1
20; 04.12.13	Nitrato de miconazol	13185611	2
AEP	Nitrato de miconazol	21000827019	1
AHC	Nitrato de miconazol	23000589004	1
AHD	Nitrato de miconazol	12374307	1
AHD	Nitrato de miconazol	21000827018	1
AHD	Nitrato de miconazol	23003273004	2
Alliance H.	Nitrato de miconazol	5137910	1
Alliance Health 05.0...	Nitrato de miconazol	13352801	2
Alliance Healthcare	Nitrato de miconazol	12374307	1
Alliance Healthcare	Nitrato de miconazol	1811015-01	2
Alliance Healthcare	Nitrato de miconazol	18C23-B02-353243	1
Alliance Healthcare	Nitrato de miconazol	18C23-B02-355295	1
Alliance	Nitrato de miconazol	22F08-B02-213149	1
Anzag	Nitrato de miconazol	12243802	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Nitrato de miconazol	12374301	3
Anzag	Nitrato de miconazol	15137902	1
Anzag	Nitrato de miconazol	15A13-B07-308432	1
Anzag	Nitrato de miconazol	16144716	1
Anzag	Nitrato de miconazol	18C23-B02-353243	1
Bionorica /Phönix	Nitrato de miconazol	12C13B03-279593	1
Bomastus / Alliance ...	Nitrato de miconazol	16E04-B03-327367	1
Bombastus	Nitrato de miconazol	13352806	1
Bombastus	Nitrato de miconazol	15I08-B07-318686	1
Bombastus	Nitrato de miconazol	15I08-B07-318687	1
Bombastus	Nitrato de miconazol	16144725	1
Caelo	Nitrato de miconazol		3
Caelo	Nitrato de miconazol	1/AD1	1
Caelo	Nitrato de miconazol	11104103	2
Caelo	Nitrato de miconazol	11104108	1
Caelo	Nitrato de miconazol	11104109	2
Caelo	Nitrato de miconazol	11104113	1
Caelo	Nitrato de miconazol	11104114	1
Caelo	Nitrato de miconazol	1122014A	1
Caelo	Nitrato de miconazol	11243803	1
Caelo	Nitrato de miconazol	11324901	1
Caelo	Nitrato de miconazol	11324902	1
Caelo	Nitrato de miconazol	11324905	4
Caelo	Nitrato de miconazol	11324909	1
Caelo	Nitrato de miconazol	11324912	2
Caelo	Nitrato de miconazol	11324913	1
Caelo	Nitrato de miconazol	122438	1
Caelo	Nitrato de miconazol	12243801	3
Caelo	Nitrato de miconazol	12243802	4
Caelo	Nitrato de miconazol	12243803	9
Caelo	Nitrato de miconazol	12243805	6
Caelo	Nitrato de miconazol	12243806	1
Caelo	Nitrato de miconazol	12243808	9
Caelo	Nitrato de miconazol	12374301	4
Caelo	Nitrato de miconazol	12374307	15
Caelo	Nitrato de miconazol	12374308	6
Caelo	Nitrato de miconazol	12k02n06	1
Caelo	Nitrato de miconazol	1307025-02	1
Caelo	Nitrato de miconazol	13185601	4
Caelo	Nitrato de miconazol	13185602	7
Caelo	Nitrato de miconazol	13185603	10
Caelo	Nitrato de miconazol	13185609	9
Caelo	Nitrato de miconazol	13185610	6
Caelo	Nitrato de miconazol	13185611	16
Caelo	Nitrato de miconazol	13185612	6
Caelo	Nitrato de miconazol	13282901	1
Caelo	Nitrato de miconazol	13342801	1
Caelo	Nitrato de miconazol	13352801	17
Caelo	Nitrato de miconazol	13352802	17
Caelo	Nitrato de miconazol	13352805	1
Caelo	Nitrato de miconazol	13352806	14
Caelo	Nitrato de miconazol	13352811	6
Caelo	Nitrato de miconazol	13D22-N14	1
Caelo	Nitrato de miconazol	13H28-N06	1
Caelo	Nitrato de miconazol	14149301	14
Caelo	Nitrato de miconazol	14149302	16
Caelo	Nitrato de miconazol	14149303	5
Caelo	Nitrato de miconazol	14149305	1
Caelo	Nitrato de miconazol	14149308	11
Caelo	Nitrato de miconazol	14149309	9

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nitrato de miconazol	14149310	9
Caelo	Nitrato de miconazol	14149311	14
Caelo	Nitrato de miconazol	14149317	10
Caelo	Nitrato de miconazol	14149318	22
Caelo	Nitrato de miconazol	1419301	1
Caelo	Nitrato de miconazol	1419310	1
Caelo	Nitrato de miconazol	14B18-B02-291233	1
Caelo	Nitrato de miconazol	14D25-B06-294959	1
Caelo	Nitrato de miconazol	14D25-B06-294960	3
Caelo	Nitrato de miconazol	14H06-B01-299799	1
Caelo	Nitrato de miconazol	15/05-B07-312317	1
Caelo	Nitrato de miconazol	15/08-B07-315481	1
Caelo	Nitrato de miconazol	151379	1
Caelo	Nitrato de miconazol	15137902	24
Caelo	Nitrato de miconazol	15137903	19
Caelo	Nitrato de miconazol	15137905	11
Caelo	Nitrato de miconazol	15137906	1
Caelo	Nitrato de miconazol	15137907	13
Caelo	Nitrato de miconazol	15137908	10
Caelo	Nitrato de miconazol	15137909	13
Caelo	Nitrato de miconazol	15137910	7
Caelo	Nitrato de miconazol	15137911	1
Caelo	Nitrato de miconazol	15137913	5
Caelo	Nitrato de miconazol	15137914	6
Caelo	Nitrato de miconazol	15137915	3
Caelo	Nitrato de miconazol	15A13-B07	1
Caelo	Nitrato de miconazol	15A13-B07-307140	1
Caelo	Nitrato de miconazol	15I08-B07-312317	3
Caelo	Nitrato de miconazol	15I08-B07-315481	1
Caelo	Nitrato de miconazol	15I08-B07-315492	1
Caelo	Nitrato de miconazol	15I08-B07-318687	2
Caelo	Nitrato de miconazol	15l08-B07-314838	1
Caelo	Nitrato de miconazol	15l08-B07-315492	1
Caelo	Nitrato de miconazol	15l08-B07-318686	1
Caelo	Nitrato de miconazol	16144701	35
Caelo	Nitrato de miconazol	16144702	27
Caelo	Nitrato de miconazol	16144703	17
Caelo	Nitrato de miconazol	16144704	14
Caelo	Nitrato de miconazol	1614471	1
Caelo	Nitrato de miconazol	16144710	17
Caelo	Nitrato de miconazol	16144711	14
Caelo	Nitrato de miconazol	16144716	30
Caelo	Nitrato de miconazol	16144717	10
Caelo	Nitrato de miconazol	16144720	10
Caelo	Nitrato de miconazol	16144721	15
Caelo	Nitrato de miconazol	16144725	38
Caelo	Nitrato de miconazol	16144726	21
Caelo	Nitrato de miconazol	16e04-b03-321367	1
Caelo	Nitrato de miconazol	16E04-B03-321367	2
Caelo	Nitrato de miconazol	16E04-B03-322124	1
Caelo	Nitrato de miconazol	16E04-B03-325448	1
Caelo	Nitrato de miconazol	16e04b03327367	1
Caelo	Nitrato de miconazol	16E04-B03-332373	1
Caelo	Nitrato de miconazol	1705039-01	2
Caelo	Nitrato de miconazol	172117505	1
Caelo	Nitrato de miconazol	1721505	1
Caelo	Nitrato de miconazol	17217053	1
Caelo	Nitrato de miconazol	17217502	52
Caelo	Nitrato de miconazol	17217503	27
Caelo	Nitrato de miconazol	17217505	32

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nitrato de miconazol	17217507	1
Caelo	Nitrato de miconazol	1727503	1
Caelo	Nitrato de miconazol	17C01B02340778	1
Caelo	Nitrato de miconazol	180057913	1
Caelo	Nitrato de miconazol	1803028-01	1
Caelo	Nitrato de miconazol	18057901	1
Caelo	Nitrato de miconazol	18057902	18
Caelo	Nitrato de miconazol	18057903	29
Caelo	Nitrato de miconazol	18057904	1
Caelo	Nitrato de miconazol	18057906	38
Caelo	Nitrato de miconazol	18057907	20
Ĉaelo	Nitrato de miconazol	18057907	1
Caelo	Nitrato de miconazol	18057909	1
Caelo	Nitrato de miconazol	18057911	1
Caelo	Nitrato de miconazol	18057912	29
Caelo	Nitrato de miconazol	18057913	34
Caelo	Nitrato de miconazol	18057914	16
Caelo	Nitrato de miconazol	18057916	1
Caelo	Nitrato de miconazol	18067907	1
Caelo	Nitrato de miconazol	1807902	1
Caelo	Nitrato de miconazol	18182111	1
Caelo	Nitrato de miconazol	1828109	1
Caelo	Nitrato de miconazol	1828113	3
Caelo	Nitrato de miconazol	182821002	1
Caelo	Nitrato de miconazol	18282101	2
Caelo	Nitrato de miconazol	18282105	32
Caelo	Nitrato de miconazol	18282106	15
Caelo	Nitrato de miconazol	18282107	2
Caelo	Nitrato de miconazol	18282108	2
Caelo	Nitrato de miconazol	18282109	29
Caelo	Nitrato de miconazol	18282110	27
Caelo	Nitrato de miconazol	18282111	29
Caelo	Nitrato de miconazol	18282113	62
Caelo	Nitrato de miconazol	18282114	19
Caelo	Nitrato de miconazol	1828213	1
Caelo	Nitrato de miconazol	18282133	1
Caelo	Nitrato de miconazol	1850000164	3
Caelo	Nitrato de miconazol	1882105	1
Caelo	Nitrato de miconazol	18B06_b03_34778	1
Caelo	Nitrato de miconazol	18B06-B03-347788	1
Caelo	Nitrato de miconazol	18C23-B02	2
Caelo	Nitrato de miconazol	18C23-B02-348857	2
Caelo	Nitrato de miconazol	18C23-B02-352488	1
Caelo	Nitrato de miconazol	18C23-B02-353243	1
Caelo	Nitrato de miconazol	18C23-B02-355707	1
Caelo	Nitrato de miconazol	19A31-B01-359396	3
Caelo	Nitrato de miconazol	19A31-B01-360614	2
Caelo	Nitrato de miconazol	200000097003	2
Caelo	Nitrato de miconazol	20000097001	1
Caelo	Nitrato de miconazol	20000097003	30
Caelo	Nitrato de miconazol	20000097004	19
Caelo	Nitrato de miconazol	20000097005	7
Caelo	Nitrato de miconazol	20000097006	13
Caelo	Nitrato de miconazol	20000097007	30
Caelo	Nitrato de miconazol	20000097009	1
Caelo	Nitrato de miconazol	2000009705	1
Caelo	Nitrato de miconazol	2000009707	1
Caelo	Nitrato de miconazol	200004304002	1
Caelo	Nitrato de miconazol	200004304003	1
Caelo	Nitrato de miconazol	2000097003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nitrato de miconazol	2000097007	1
Caelo	Nitrato de miconazol	20001304002	1
Caelo	Nitrato de miconazol	20004304001	1
Caelo	Nitrato de miconazol	20004304002	18
Caelo	Nitrato de miconazol	20004304003	44
Caelo	Nitrato de miconazol	20004304004	1
Caelo	Nitrato de miconazol	20004304006	3
Caelo	Nitrato de miconazol	2004304002	2
Caelo	Nitrato de miconazol	2004304003	1
Caelo	Nitrato de miconazol	2100027013	1
Caelo	Nitrato de miconazol	21000827	1
Caelo	Nitrato de miconazol	21000827001	2
Caelo	Nitrato de miconazol	21000827002	14
Caelo	Nitrato de miconazol	21000827003	49
Caelo	Nitrato de miconazol	21000827006	12
Caelo	Nitrato de miconazol	21000827007	3
Caelo	Nitrato de miconazol	21000827008	24
Caelo	Nitrato de miconazol	21000827010	5
Caelo	Nitrato de miconazol	21000827011	7
Caelo	Nitrato de miconazol	21000827012	5
Caelo	Nitrato de miconazol	21000827013	15
Caelo	Nitrato de miconazol	21000827014	19
Caelo	Nitrato de miconazol	21000827015	9
Caelo	Nitrato de miconazol	21000827016	7
Caelo	Nitrato de miconazol	21000827017	6
Caelo	Nitrato de miconazol	21000827019	4
Caelo	Nitrato de miconazol	21000827021	3
Caelo	Nitrato de miconazol	21000827022	5
Caelo	Nitrato de miconazol	21000827023	1
Caelo	Nitrato de miconazol	21000827024	5
Caelo	Nitrato de miconazol	21000827025	1
Caelo	Nitrato de miconazol	21000827026	3
Caelo	Nitrato de miconazol	21000827103	1
Caelo	Nitrato de miconazol	2100827002	1
Caelo	Nitrato de miconazol	2100827003	1
Caelo	Nitrato de miconazol	2100827008	2
Caelo	Nitrato de miconazol	2100827014	1
Caelo	Nitrato de miconazol	2100827019	1
Caelo	Nitrato de miconazol	2103012-01	3
Caelo	Nitrato de miconazol	211019(20004304002)	1
Caelo	Nitrato de miconazol	211020(21000827002)	1
Caelo	Nitrato de miconazol	21C09-F01-377510	1
Caelo	Nitrato de miconazol	21C09-F01-3775100	2
Caelo	Nitrato de miconazol	220004304003	1
Caelo	Nitrato de miconazol	2747	1
Caelo	Nitrato de miconazol	2773	1
Caelo	Nitrato de miconazol	2777	1
Caelo	Nitrato de miconazol	2787	1
Caelo	Nitrato de miconazol	2796	1
Caelo	Nitrato de miconazol	28051306	1
Caelo	Nitrato de miconazol	2900/10/14	1
Caelo	Nitrato de miconazol	2900/11/15	3
Caelo	Nitrato de miconazol	29001614	1
Caelo	Nitrato de miconazol	4061304	1
Caelo	Nitrato de miconazol	411092-2-P	1
Caelo	Nitrato de miconazol	8/AKD4	1
Caelo	Nitrato de miconazol	818A-03451	1
Caelo	Nitrato de miconazol	8704870	1
Caelo	Nitrato de miconazol	8716	1
Caelo	Nitrato de miconazol	9177904	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nitrato de miconazol	AKD9	1
Caelo	Nitrato de miconazol	F04-3700307	2
Caesar & Lorenz GmbH	Nitrato de miconazol	18282113	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282111	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282110	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282113	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097004	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827003	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827017	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827008	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827022	2
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827003	2
Caesar & Loretz GmbH...	Nitrato de miconazol	14149301	1
Caesar & Loretz GmbH...	Nitrato de miconazol	11324904	1
Caesar & Loretz GmbH...	Nitrato de miconazol	13185602	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282111	2
Caesar & Loretz GmbH...	Nitrato de miconazol	18057914	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282106	2
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827021	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282105	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282105	1
Caesar & Loretz GmbH...	Nitrato de miconazol	2000009703	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282111	1
Caesar & Loretz GmbH/AHD	Nitrato de miconazol	20000097003	1
Caesar & Loretz GmbH/AHD	Nitrato de miconazol	21000827003	1
Caesar & Loretz GmbH/AHD	Nitrato de miconazol	21000827022	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18057906	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20004304003	2
Caesar & Loretz GmbH/G	Nitrato de miconazol	20004304003	1
Caesar & Loretz GmbH/Gehe	Nitrato de miconazol	20000097003	1
Caesar & Loretz GmbH/Gehe	Nitrato de miconazol	20004304002	1
Caesar & Loretz GmbH/Gehe	Nitrato de miconazol	21000827013	1
Caesar & Loretz GmbH/Gehe	Nitrato de miconazol	21000827016	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097007	2
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097004	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18057913	1
Caesar & Loretz GmbH...	Nitrato de miconazol	182821002	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282113	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097004	2
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097009	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20004304003	2
Caesar & Loretz GmbH...	Nitrato de miconazol	20004304004	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827001	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20004304001	1
Caesar & Loretz GmbH...	Nitrato de miconazol	18282113	2
Caesar & Loretz GmbH...	Nitrato de miconazol	18282114	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827014	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827019	1
Caesar & Loretz GmbH...	Nitrato de miconazol		1
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097004	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097007	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20004304002	2
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827003	1
Caesar & Loretz GmbH/S	Nitrato de miconazol	21000827008	2
Caesar & Loretz GmbH...	Nitrato de miconazol	18282105	2
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097004	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20000097005	1
Caesar & Loretz GmbH...	Nitrato de miconazol	20004304003	1
Caesar & Loretz GmbH...	Nitrato de miconazol	21000827003	2
Caesar & Loretz GmbH...	Nitrato de miconazol	18282105	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Nitrato de miconazol	16144702	1
Caesar & Loretz GmbH	Nitrato de miconazol	16144717	1
Caesar & Loretz GmbH	Nitrato de miconazol	18057906	3
Caesar & Loretz GmbH	Nitrato de miconazol	18057912	3
Caesar & Loretz GmbH	Nitrato de miconazol	18057913	12
Caesar & Loretz GmbH	Nitrato de miconazol	18057914	1
Caesar & Loretz GmbH	Nitrato de miconazol	18100226	1
Caesar & Loretz GmbH	Nitrato de miconazol	182821002	3
Caesar & Loretz GmbH	Nitrato de miconazol	18282105	7
Caesar & Loretz GmbH	Nitrato de miconazol	18282106	2
Caesar & Loretz GmbH	Nitrato de miconazol	18282108	2
Caesar & Loretz GmbH	Nitrato de miconazol	18282109	15
Caesar & Loretz GmbH	Nitrato de miconazol	18282110	7
Caesar & Loretz GmbH	Nitrato de miconazol	18282111	5
Caesar & Loretz GmbH	Nitrato de miconazol	18282112	1
Caesar & Loretz GmbH	Nitrato de miconazol	18282113	17
Caesar & Loretz GmbH	Nitrato de miconazol	18282114	7
Caesar & Loretz GmbH	Nitrato de miconazol	19J16-F02	1
Caesar & Loretz GmbH	Nitrato de miconazol	20000097002	1
Caesar & Loretz GmbH	Nitrato de miconazol	20000097003	8
Caesar & Loretz GmbH	Nitrato de miconazol	20000097004	4
Caesar & Loretz GmbH	Nitrato de miconazol	20000097005	7
Caesar & Loretz GmbH	Nitrato de miconazol	20000097006	4
Caesar & Loretz GmbH	Nitrato de miconazol	20000097007	15
Caesar & Loretz GmbH	Nitrato de miconazol	20000097009	1
Caesar & Loretz GmbH	Nitrato de miconazol	2000097004	1
Caesar & Loretz GmbH	Nitrato de miconazol	20004304001	2
Caesar & Loretz GmbH	Nitrato de miconazol	20004304002	3
Caesar & Loretz GmbH	Nitrato de miconazol	20004304003	9
Caesar & Loretz GmbH	Nitrato de miconazol	20004304004	2
Caesar & Loretz GmbH	Nitrato de miconazol	21000827001	3
Caesar & Loretz GmbH	Nitrato de miconazol	21000827002	9
Caesar & Loretz GmbH	Nitrato de miconazol	21000827003	12
Caesar & Loretz GmbH	Nitrato de miconazol	21000827006	3
Caesar & Loretz GmbH	Nitrato de miconazol	21000827008	5
Caesar & Loretz GmbH	Nitrato de miconazol	21000827009	2
Caesar & Loretz GmbH	Nitrato de miconazol	21000827010	3
Caesar & Loretz GmbH	Nitrato de miconazol	21000827011	4
Caesar & Loretz GmbH	Nitrato de miconazol	21000827013	4
Caesar & Loretz GmbH	Nitrato de miconazol	21000827014	2
Caesar & Loretz GmbH	Nitrato de miconazol	21000827015	4
Caesar & Loretz GmbH	Nitrato de miconazol	21000827016	3
Caesar & Loretz GmbH	Nitrato de miconazol	21000827017	4
Caesar & Loretz GmbH	Nitrato de miconazol	21000827021	2
Caesar & Loretz GmbH	Nitrato de miconazol	21000827023	1
Caesar & Loretz GmbH	Nitrato de miconazol	F01-3775100	1
Caesar & Loretz Hilden	Nitrato de miconazol	18057912	1
Caesar & Loretz Hilden	Nitrato de miconazol	18057913	1
Caesar & Loretz Hilden	Nitrato de miconazol	18282110	1
Caesar & Loretz Hilden	Nitrato de miconazol	18282113	3
Caesar & Loretz Hilden	Nitrato de miconazol	20000097003	1
Caesar & Loretz Hilden	Nitrato de miconazol	20000097007	1
Caesar & Loretz/AHC	Nitrato de miconazol	15137910	1
Caesar & Loretz/Geil...	Nitrato de miconazol	20000097003	2
Caesar & Loretz/Geil...	Nitrato de miconazol	20000097004	1
Caesar & Loretz/Geil...	Nitrato de miconazol	20000097007	1
Caesar & Loretz	Nitrato de miconazol	16144724	1
Caesar & Loretz	Nitrato de miconazol	18282109	2
Caesar & Loretz	Nitrato de miconazol	1850000164	1
Caesar Loretz Gehe	Nitrato de miconazol	21000827008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar und Loretz	Nitrato de miconazol	12243805	1
Caesar&Lorenz	Nitrato de miconazol	20004304002	1
Caesar&Loretz GmbH ...	Nitrato de miconazol	12243808	1
Caesar&Loretz GmbH /Anzag	Nitrato de miconazol	14149310	1
Caesar&Loretz GmbH/Anzag	Nitrato de miconazol	13185603	1
Caesar&Loretz GmbH/Anzag	Nitrato de miconazol	13352802	1
Caesar&loretz,Phoenix	Nitrato de miconazol	12374301	1
Cealo / Otto Geilenk...	Nitrato de miconazol	18282106	1
Cealo / Otto Geilenk...	Nitrato de miconazol	18282111	1
Cealo/Gehe	Nitrato de miconazol	20000097007	1
Dr. Wolff	Nitrato de miconazol	18E04-B03	1
E+J, 27.09.2016	Nitrato de miconazol	15137915	1
Ebert & Jacobi	Nitrato de miconazol	15137914	1
Erregierre / Gehe	Nitrato de miconazol	18282114	1
Erregierre IT/Noweda	Nitrato de miconazol	15137905	1
Erregierre spa	Nitrato de miconazol	18282111	1
Erregierre/Noweda	Nitrato de miconazol	A180001	1
Erregierre/Noweda	Nitrato de miconazol	A190001	1
EuRho/ AHD	Nitrato de miconazol	16E04-B03-332373	1
EuRho	Nitrato de miconazol	161102401	1
EuRho	Nitrato de miconazol	1705039-01	2
euRho	Nitrato de miconazol	2009034-01	1
Eurho	Nitrato de miconazol	2103012-01	1
euro AHD	Nitrato de miconazol	1710020-015633	1
euro AHD	Nitrato de miconazol	1710020-015639	1
Euro OTC	Nitrato de miconazol	1307025-01	2
Euro OTC	Nitrato de miconazol	1307025-02	2
Euro OTC	Nitrato de miconazol	140902301	1
Euro OTC	Nitrato de miconazol	1409023-01	1
Euro OTC	Nitrato de miconazol	140902302	1
Euro OTC	Nitrato de miconazol	1409023-02	4
Euro OTC	Nitrato de miconazol	1504003-01	2
Euro OTC	Nitrato de miconazol	1504903-01	1
Euro OTC	Nitrato de miconazol	1509014-01	6
Euro OTC	Nitrato de miconazol	1604004-01	5
Euro OTC	Nitrato de miconazol	1607004-01	9
Euro OTC	Nitrato de miconazol	1611024-01	12
Euro OTC	Nitrato de miconazol	1611024-015307	1
Euro OTC	Nitrato de miconazol	1611024-015330	1
Euro OTC	Nitrato de miconazol	1611024-02	3
Euro OTC	Nitrato de miconazol	16144701	1
Euro OTC	Nitrato de miconazol	16E04-B03-322124	1
Euro OTC	Nitrato de miconazol	16E04-B03-327362	2
Euro OTC	Nitrato de miconazol	170503901	1
Euro OTC	Nitrato de miconazol	1705039-01	12
Euro OTC	Nitrato de miconazol	1705039-015371	1
Euro OTC	Nitrato de miconazol	1705039-015432	1
Euro OTC	Nitrato de miconazol	1705039-02	6
Euro OTC	Nitrato de miconazol	1710020-01	9
Euro OTC	Nitrato de miconazol	1710020-015457	1
Euro OTC	Nitrato de miconazol	17C01-B02-339699	1
Euro OTC	Nitrato de miconazol	17C01-B02-341814	1
Euro OTC	Nitrato de miconazol	1803028-01	23
Euro OTC	Nitrato de miconazol	18057907	1
Euro OTC	Nitrato de miconazol	18057912	1
Euro OTC	Nitrato de miconazol	1811015	1
Euro OTC	Nitrato de miconazol	181101501	1
Euro OTC	Nitrato de miconazol	1811015-01	22
Euro OTC	Nitrato de miconazol	1850003395	1
Euro OTC	Nitrato de miconazol	19009029-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nitrato de miconazol	1904032-01	1
Euro OTC	Nitrato de miconazol	1909029-01	21
Euro OTC	Nitrato de miconazol	190929-01	1
Euro OTC	Nitrato de miconazol	1950000070	1
Euro OTC	Nitrato de miconazol	1950001767	1
Euro OTC	Nitrato de miconazol	19A31-B01-359397	1
Euro OTC	Nitrato de miconazol	2009034-01	23
Euro OTC	Nitrato de miconazol	200903402	1
Euro OTC	Nitrato de miconazol	2009034-02	4
Euro OTC	Nitrato de miconazol	2009034-03	3
Euro OTC	Nitrato de miconazol	20180430/5	1
Euro OTC	Nitrato de miconazol	21000827014	1
Euro OTC	Nitrato de miconazol	210301201	2
Euro OTC	Nitrato de miconazol	2103012-01	21
Euro OTC	Nitrato de miconazol	2103012-02	3
Euro OTC	Nitrato de miconazol	2103912-02	1
Euro OTC	Nitrato de miconazol	2150000385	1
Euro OTC	Nitrato de miconazol	22100002-01	1
Euro OTC	Nitrato de miconazol	2210002-01	6
Euro OTC	Nitrato de miconazol	F02-3670602	1
Euro/Phönix	Nitrato de miconazol	1803028-01	3
EuroPTC/Phönix	Nitrato de miconazol	14149316	1
Fagron	Nitrato de miconazol		1
Fagron	Nitrato de miconazol	12/21-M03	1
Fagron	Nitrato de miconazol	12A16-N02	2
Fagron	Nitrato de miconazol	12H10-N02	4
Fagron	Nitrato de miconazol	12K02-N06	5
Fagron	Nitrato de miconazol	13061501	1
Fagron	Nitrato de miconazol	1316Q-03451	1
Fagron	Nitrato de miconazol	1328-N06	1
Fagron	Nitrato de miconazol	13A14-B09	2
Fagron	Nitrato de miconazol	13A14B09283005	1
Fagron	Nitrato de miconazol	13A14-B09-287453	1
Fagron	Nitrato de miconazol	13A14-B09-287486	5
Fagron	Nitrato de miconazol	13A14-B09-287487	3
Fagron	Nitrato de miconazol	13A14-B09-287488	1
Fagron	Nitrato de miconazol	13D22-N14	6
Fagron	Nitrato de miconazol	13E13-N04	2
Fagron	Nitrato de miconazol	13E13-N08	2
Fagron	Nitrato de miconazol	13H28_N06	1
Fagron	Nitrato de miconazol	13H28-N06	13
Fagron	Nitrato de miconazol	13H28-NO6	2
Fagron	Nitrato de miconazol	14051403	1
Fagron	Nitrato de miconazol	14149313	1
Fagron	Nitrato de miconazol	14B18B02	1
Fagron	Nitrato de miconazol	14B18-B02	4
Fagron	Nitrato de miconazol	14b18-B02-291231	1
Fagron	Nitrato de miconazol	14B18-B02-291232	4
Fagron	Nitrato de miconazol	14b18-b02-291247	1
Fagron	Nitrato de miconazol	14B18-B02-291247	2
Fagron	Nitrato de miconazol	14B18-B02-291248	7
Fagron	Nitrato de miconazol	14B18-B02-291249	1
Fagron	Nitrato de miconazol	14B18-B02-291250	1
Fagron	Nitrato de miconazol	14D25-B06	4
Fagron	Nitrato de miconazol	14D25-B06-294958	15
Fagron	Nitrato de miconazol	14D25-B06-294959	8
Fagron	Nitrato de miconazol	14d25-b06-294960	1
Fagron	Nitrato de miconazol	14D25-B06-294960	1
Fagron	Nitrato de miconazol	14d25-b06-299790	1
Fagron	Nitrato de miconazol	14D25-B06-299790	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Nitrato de miconazol	14H06-B01-299798	1
Fagron	Nitrato de miconazol	14H06-B01-299799	8
Fagron	Nitrato de miconazol	14H06-B01-299813	5
Fagron	Nitrato de miconazol	14H16-B01-299798	1
Fagron	Nitrato de miconazol	15/08-B07-312317	2
Fagron	Nitrato de miconazol	15/08-b07-314838	2
Fagron	Nitrato de miconazol	15/08-B07-314838	2
Fagron	Nitrato de miconazol	15/08-B07-315481	1
Fagron	Nitrato de miconazol	15/08-b07-315492	2
Fagron	Nitrato de miconazol	15/08-B07-316911	1
Fagron	Nitrato de miconazol	15/08-B07-318686	3
Fagron	Nitrato de miconazol	15/08-b07-318687	1
Fagron	Nitrato de miconazol	1508-B07-314838	1
Fagron	Nitrato de miconazol	1508-B07-318686	1
Fagron	Nitrato de miconazol	15108-b07-312321	1
Fagron	Nitrato de miconazol	15108-B07-318485	1
Fagron	Nitrato de miconazol	15137905	1
Fagron	Nitrato de miconazol	15137915	1
Fagron	Nitrato de miconazol	15A13-807	1
Fagron	Nitrato de miconazol	15A13-B07	7
Fagron	Nitrato de miconazol	15A13-B07-306565	1
Fagron	Nitrato de miconazol	15A13-B07-306791	11
Fagron	Nitrato de miconazol	15A13-B07-306791nron	1
Fagron	Nitrato de miconazol	15a13-b07-307140	1
Fagron	Nitrato de miconazol	15A13-B07-307140	11
Fagron	Nitrato de miconazol	15a13-b07-308432	1
Fagron	Nitrato de miconazol	15A13-B07-308432	4
Fagron	Nitrato de miconazol	15I08-B07	3
Fagron	Nitrato de miconazol	15I08-B07-215492	1
Fagron	Nitrato de miconazol	15I08-B07-3121321	1
Fagron	Nitrato de miconazol	15i08-b07-312317	1
Fagron	Nitrato de miconazol	15I08-B07-312317	3
Fagron	Nitrato de miconazol	15I08-B07-312321	11
Fagron	Nitrato de miconazol	15I08-B07-314838	2
Fagron	Nitrato de miconazol	15I08-B07-31485	1
Fagron	Nitrato de miconazol	15i08-b07-315481	1
Fagron	Nitrato de miconazol	15I08-B07-315481	2
Fagron	Nitrato de miconazol	15I08-B07-315492	2
Fagron	Nitrato de miconazol	15I08-B07-318485	3
Fagron	Nitrato de miconazol	15I08-B07-318686	2
Fagron	Nitrato de miconazol	15I08-B07-318687	2
Fagron	Nitrato de miconazol	15I18-B07-318485	1
Fagron	Nitrato de miconazol	15l08-B07-312321	1
Fagron	Nitrato de miconazol	15l08-B07-315492	3
Fagron	Nitrato de miconazol	15l08-B07-318686	1
Fagron	Nitrato de miconazol	160711M	1
Fagron	Nitrato de miconazol	16144702	1
Fagron	Nitrato de miconazol	16144703	1
Fagron	Nitrato de miconazol	16144725	2
Fagron	Nitrato de miconazol	16E04-B03	8
Fagron	Nitrato de miconazol	16E04-B03-321354	3
Fagron	Nitrato de miconazol	16E04-B03-321367	2
Fagron	Nitrato de miconazol	16E04-B03-322124	15
Fagron	Nitrato de miconazol	16e04-b03-322131	2
Fagron	Nitrato de miconazol	16E04-B03-322131	9
Fagron	Nitrato de miconazol	16E04-B03-322132	8
Fagron	Nitrato de miconazol	16E04-B03-327362	9
Fagron	Nitrato de miconazol	16E04-B03-327367	1
Fagron	Nitrato de miconazol	16E04-B03-330082	9
Fagron	Nitrato de miconazol	16E04-B03-332373	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Nitrato de miconazol	17011307	1
Fagron	Nitrato de miconazol	17C01B02	1
Fagron	Nitrato de miconazol	17C01-B02	6
Fagron	Nitrato de miconazol	17C01-B02-225671	1
Fagron	Nitrato de miconazol	17c01-b02-334877	1
Fagron	Nitrato de miconazol	17C01-B02-334877	8
Fagron	Nitrato de miconazol	17C01-B02-334882	4
Fagron	Nitrato de miconazol	17c01-b02-335671	1
Fagron	Nitrato de miconazol	17C01-B02-335671	6
Fagron	Nitrato de miconazol	17C01-B02-338798	3
Fagron	Nitrato de miconazol	17c01-b02-340778	1
Fagron	Nitrato de miconazol	17C01-B02-340778	15
Fagron	Nitrato de miconazol	17C01-B02-341395	4
Fagron	Nitrato de miconazol	1811015-01	1
Fagron	Nitrato de miconazol	1850000164	4
Fagron	Nitrato de miconazol	1850003395	4
Fagron	Nitrato de miconazol	18B06-B03	5
Fagron	Nitrato de miconazol	18b06-b03-345419	1
Fagron	Nitrato de miconazol	18B06-B03-345419	10
Fagron	Nitrato de miconazol	18B06-B03-345422	5
Fagron	Nitrato de miconazol	18b06-b03-345423	2
Fagron	Nitrato de miconazol	18B06-B03-345423	5
Fagron	Nitrato de miconazol	18b06-b03-347788	1
Fagron	Nitrato de miconazol	18B06-B03-347788	4
Fagron	Nitrato de miconazol	18c23-b02	1
Fagron	Nitrato de miconazol	18C23-B02	11
Fagron	Nitrato de miconazol	18C23-B02-248857	1
Fagron	Nitrato de miconazol	18C23-B02-347802	6
Fagron	Nitrato de miconazol	18c23-b02-348857	1
Fagron	Nitrato de miconazol	18C23-B02-348857	3
Fagron	Nitrato de miconazol	18C23-B02-350961	3
Fagron	Nitrato de miconazol	18C23-B02-351310	10
Fagron	Nitrato de miconazol	18C23-B02-352488	5
Fagron	Nitrato de miconazol	18c23-b02-352489	1
Fagron	Nitrato de miconazol	18C23-B02-352489	5
Fagron	Nitrato de miconazol	18C23-B02-353243	8
Fagron	Nitrato de miconazol	18c23-b02-354469	1
Fagron	Nitrato de miconazol	18C23-B02-354469	5
Fagron	Nitrato de miconazol	18C23-B02-355295	5
Fagron	Nitrato de miconazol	18c23-b02-355707	1
Fagron	Nitrato de miconazol	18C23-B02-355707	7
Fagron	Nitrato de miconazol	18C23-B02-356141	5
Fagron	Nitrato de miconazol	18C-B02-354469	1
Fagron	Nitrato de miconazol	19041705	1
Fagron	Nitrato de miconazol	19051402	1
Fagron	Nitrato de miconazol	19500002545P-200709	1
Fagron	Nitrato de miconazol	1950002545	6
Fagron	Nitrato de miconazol	19A31-B01	11
Fagron	Nitrato de miconazol	19A31B0132992	1
Fagron	Nitrato de miconazol	19A31-B01-358150	3
Fagron	Nitrato de miconazol	19A31-B01-359391	2
Fagron	Nitrato de miconazol	19A31-b01-359392	1
Fagron	Nitrato de miconazol	19A31-B01-359392	17
Fagron	Nitrato de miconazol	19A31B01359396	1
Fagron	Nitrato de miconazol	19A31-B01-359396	5
Fagron	Nitrato de miconazol	19A31-B01-359397	8
Fagron	Nitrato de miconazol	19A31-B01-360612	5
Fagron	Nitrato de miconazol	19A31-B01-360613	6
Fagron	Nitrato de miconazol	19A31-B01-360614	2
Fagron	Nitrato de miconazol	19A31-B01-359392	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Nitrato de miconazol	19F16-F02-366310	1
Fagron	Nitrato de miconazol	19J16-F01-367062	1
Fagron	Nitrato de miconazol	19J16-F02	7
Fagron	Nitrato de miconazol	19J16-F02-366299	1
Fagron	Nitrato de miconazol	19J16-F02-366300	8
Fagron	Nitrato de miconazol	19J16-F02366310	1
Fagron	Nitrato de miconazol	19J16-F02-366310	7
Fagron	Nitrato de miconazol	19J16-F02-3663100	1
Fagron	Nitrato de miconazol	19J16-F02-366311	14
Fagron	Nitrato de miconazol	19J16-F02-3670603	1
Fagron	Nitrato de miconazol	19J16-F02-367062	9
Fagron	Nitrato de miconazol	19J16-F02-367063	6
Fagron	Nitrato de miconazol	19J16-F02-367064	1
Fagron	Nitrato de miconazol	19J16-F02-37062	1
Fagron	Nitrato de miconazol	20081201	1
Fagron	Nitrato de miconazol	2050000157	7
Fagron	Nitrato de miconazol	20B21-04-376344	1
Fagron	Nitrato de miconazol	20B21-F04	2
Fagron	Nitrato de miconazol	20B21-F04-370036	2
Fagron	Nitrato de miconazol	20B21-F04-370037	15
Fagron	Nitrato de miconazol	20B21-F04-370040	3
Fagron	Nitrato de miconazol	20B21-F04-3700400	1
Fagron	Nitrato de miconazol	20B21-F04-370270	8
Fagron	Nitrato de miconazol	20B21-F04-376344	6
Fagron	Nitrato de miconazol	2150000385	3
Fagron	Nitrato de miconazol	21C09-F01	5
Fagron	Nitrato de miconazol	21C09-F01-277510	1
Fagron	Nitrato de miconazol	21C09-F01-37510	1
Fagron	Nitrato de miconazol	21C09-F01-37513	1
Fagron	Nitrato de miconazol	21C09-F01-377509	1
Fagron	Nitrato de miconazol	21C09-F01-377510	11
Fagron	Nitrato de miconazol	21C09-F01-377510/215000038	1
Fagron	Nitrato de miconazol	21C09-F01-377513	5
Fagron	Nitrato de miconazol	22F08_B02_213580	1
Fagron	Nitrato de miconazol	22F08-B02	2
Fagron	Nitrato de miconazol	22f08-b02-213149	1
Fagron	Nitrato de miconazol	22F08-B02-213149	14
Fagron	Nitrato de miconazol	22F-08-B02-213149	1
Fagron	Nitrato de miconazol	22F08B02213580	1
Fagron	Nitrato de miconazol	22F08-B02-221067	5
Fagron	Nitrato de miconazol	22F08B02213580	1
Fagron	Nitrato de miconazol	2366310	1
Fagron	Nitrato de miconazol	27061202	1
Fagron	Nitrato de miconazol	2900/03/16	2
Fagron	Nitrato de miconazol	2900/04/14	2
Fagron	Nitrato de miconazol	2900/08/12	2
Fagron	Nitrato de miconazol	2900/09/16	4
Fagron	Nitrato de miconazol	2900/10/14	1
Fagron	Nitrato de miconazol	2900/11/15	2
Fagron	Nitrato de miconazol	2900/15/13	2
Fagron	Nitrato de miconazol	2900/16/14	4
Fagron	Nitrato de miconazol	2900-03-16	1
Fagron	Nitrato de miconazol	29091808	1
Fagron	Nitrato de miconazol	20B21-F04-3700400	1
Fagron	Nitrato de miconazol	31101306	1
Fagron	Nitrato de miconazol	3248	1
Fagron	Nitrato de miconazol	4111301	1
Fagron	Nitrato de miconazol	8568674	1
Fagron	Nitrato de miconazol	B01-3593902	1
Fagron	Nitrato de miconazol	B01-3593906	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Nitrato de miconazol	B01-359396	1
Fagron	Nitrato de miconazol	B01-3606104	1
Fagron	Nitrato de miconazol	F01-377510	1
Fagron	Nitrato de miconazol	F02-3670602	1
Fagron	Nitrato de miconazol	F04-3700307	2
Fagron	Nitrato de miconazol	F04-3700400	1
Fagron	Nitrato de miconazol	F04-3763404	1
Fargon/Phönix	Nitrato de miconazol	19J16-F02-367063	1
Fargon	Nitrato de miconazol	14D25-B06-294959	1
Fargon	Nitrato de miconazol	18B06-B03-345423	1
Fargon	Nitrato de miconazol	22F08-B02-213149	1
Faron	Nitrato de miconazol	19A31-B01-359397	1
Fiebig	Nitrato de miconazol	15/08-B07-314838	1
Fiebig	Nitrato de miconazol	16144726	1
Fischar / Geilenkirchen	Nitrato de miconazol	16144726	1
Fragon	Nitrato de miconazol	18C23-B02-348857	1
GEHE 13.05	Nitrato de miconazol	14149311	1
Gehe 6.03.15	Nitrato de miconazol	14149308	2
Gehe am 29.04.2014	Nitrato de miconazol	13352802	4
Gehe/Ichthyol	Nitrato de miconazol	16E04-B03-322132	1
Gehe	Nitrato de miconazol	13352811	1
Gehe	Nitrato de miconazol	14149301	1
Gehe	Nitrato de miconazol	16144702	1
Gehe	Nitrato de miconazol	16144704	1
Gehe	Nitrato de miconazol	16144711	1
GEHE	Nitrato de miconazol	16144716	1
Gehe	Nitrato de miconazol	16144720	1
Gehe	Nitrato de miconazol	16E04-B03-327362	1
GEHE	Nitrato de miconazol	18057903	1
Gehe	Nitrato de miconazol	18282105	1
Gehe	Nitrato de miconazol	18B06-B03-345419	1
Gehe	Nitrato de miconazol	20000097005	1
Gehe	Nitrato de miconazol	21000827003	1
Gehe	Nitrato de miconazol	21000827008	2
Gehe	Nitrato de miconazol	21000827016	1
Gehe	Nitrato de miconazol	21000827023	1
Gehe	Nitrato de miconazol	21000827025	2
Gehe	Nitrato de miconazol	210301201	1
Gehe	Nitrato de miconazol	22F08-B02-221067	3
gehe-06.11.18	Nitrato de miconazol	18057906	1
Geibo/Noweda	Nitrato de miconazol	17217503	1
Geilenkirchen	Nitrato de miconazol	17217505	3
Geilenkirchen	Nitrato de miconazol	18057914	1
Hedinger	Nitrato de miconazol	16144720	2
Hedinger	Nitrato de miconazol	P2018/114	1
Herstellung	Nitrato de miconazol	13185602	1
Ichthyol/Phoenix	Nitrato de miconazol	16/098/M	1
Jenne	Nitrato de miconazol	21000827002	1
Kehr	Nitrato de miconazol	17C01-B02-334877	1
Kehr	Nitrato de miconazol	21000827022	2
Kehr	Nitrato de miconazol	21000827024	3
Kehr	Nitrato de miconazol	22F08-B02	1
Kehr	Nitrato de miconazol	23000589004	1
Miconazolnitrat	Nitrato de miconazol	20B21-F04-376344	1
Noveda	Nitrato de miconazol	18282105	1
Noweda 10.12.2019	Nitrato de miconazol	18282106	1
Noweda 26.11.2019	Nitrato de miconazol	18282111	1
Noweda	Nitrato de miconazol		1
Noweda	Nitrato de miconazol	14149310	1
Noweda	Nitrato de miconazol	14149311	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Nitrato de miconazol	15137903	1
Noweda	Nitrato de miconazol	16144704	1
Noweda	Nitrato de miconazol	16144721	1
Noweda	Nitrato de miconazol	16E04-B03-322124	1
Noweda	Nitrato de miconazol	1705039-02	1
Noweda	Nitrato de miconazol	17217502	1
Noweda	Nitrato de miconazol	17217505	1
Noweda	Nitrato de miconazol	18057913	1
Noweda	Nitrato de miconazol	18282109	1
Noweda	Nitrato de miconazol	18282113	1
Noweda	Nitrato de miconazol	19A31-B01-359392	3
Noweda	Nitrato de miconazol	20000097003	1
Noweda	Nitrato de miconazol	21000827008	1
Noweda	Nitrato de miconazol	21000827013	1
Noweda	Nitrato de miconazol	21000827022	1
Noweda	Nitrato de miconazol	22F08-B02	1
Olon (Lodiagiano)/Sa...	Nitrato de miconazol	2050000157	1
Otto Geilenkirchen	Nitrato de miconazol	21000827024	1
Phoenix 21.10.14	Nitrato de miconazol	14149301	1
Phoenix	Nitrato de miconazol	13185611	1
Phoenix	Nitrato de miconazol	13352801	1
Phoenix	Nitrato de miconazol	15137915	1
Phoenix	Nitrato de miconazol	15E04-B03-327367	1
Phoenix	Nitrato de miconazol	17C01-B02-334882	1
Phoenix	Nitrato de miconazol	18C23-B02-352489	1
Phoenix	Nitrato de miconazol	22110002-01	1
Phoenix	Nitrato de miconazol	23000589004	1
Phoenix	Nitrato de miconazol	B01-3606104	1
PhoenixWE: 28.04.18 ...	Nitrato de miconazol	17217505	1
Phönix	Nitrato de miconazol	13H28-N06	1
phönix	Nitrato de miconazol	15137907	1
phönix	Nitrato de miconazol	16144701	2
phönix	Nitrato de miconazol	16144716	1
Phönix	Nitrato de miconazol	16E04-B03-322124	1
Phönix	Nitrato de miconazol	16E04-B03-322131	1
Phönix	Nitrato de miconazol	17217502	2
Phönix	Nitrato de miconazol	18C23-B02-355707	1
Phönix	Nitrato de miconazol	1909029-01	1
Phönix	Nitrato de miconazol	2009034-01	1
Phönix	Nitrato de miconazol	20B21f04376344	1
Phönix	Nitrato de miconazol	20B21-F04-376344	1
Phönix	Nitrato de miconazol	21000827026	2
Phönix	Nitrato de miconazol	2103012-01	1
Phönix	Nitrato de miconazol	2210002-01	1
Phönix	Nitrato de miconazol	3133	1
Sanacop	Nitrato de miconazol		1
Sanacorp EK:5,95 ...	Nitrato de miconazol	16144703	1
Sanacorp W.E:27.03.1...	Nitrato de miconazol	16144726	2
Sanacorp	Nitrato de miconazol		1
Sanacorp	Nitrato de miconazol	12243801	1
Sanacorp	Nitrato de miconazol	12243803	2
Sanacorp	Nitrato de miconazol	13352801	1
Sanacorp	Nitrato de miconazol	16144720	1
Sanacorp	Nitrato de miconazol	18057903	1
Sanacorp	Nitrato de miconazol	18057912	1
Sanacorp	Nitrato de miconazol	18057913	1
Sanacorp	Nitrato de miconazol	18282107	1
Sanacorp	Nitrato de miconazol	18282108	1
Sanacorp	Nitrato de miconazol	18282109	2
Sanacorp	Nitrato de miconazol	18282112	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Nitrato de miconazol	18282113	1
Sanacorp	Nitrato de miconazol	18C23-B02-351310	1
Sanacorp	Nitrato de miconazol	21000827006	1
Sanacorp	Nitrato de miconazol	21000827008	1
Sanacorp	Nitrato de miconazol	21000827011	1
Sanacorp	Nitrato de miconazol	21000827015	1
Sanacorp	Nitrato de miconazol	21000827023	1
Sanacorp	Nitrato de miconazol	21000837088	1
Sanacorp	Nitrato de miconazol	2210002-01	1
Sanacorp	Nitrato de miconazol	22Fo8-B02-221067	1
Sanacorp	Nitrato de miconazol	2900/09/16	1

- 232 811 spectra from 1515 *Apo-Ident* customers from a total of 48 755 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nitrato de miconazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nitrato de miconazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	499	0	152 463
Type B	0	670	0	201 414
Type C	0	3249	7	232 811

The substance/substance group *Nitrato de miconazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7976 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1045 %)
Type C	100.0000 % (> 99.9007 %)	99.7850 % (> 99.6929 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20817	21900	6,37	53,18
20875	21350	8,51	53,35
20905	21900	7,76	46,84
21350	21350	0,00	52,46
21351	21350	2,77	51,09
21649	21900	6,91	51,71
21900	21900	0,00	53,94
22630	22630	0,00	54,91
24593	21900	6,74	53,51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nitrato de nafazolina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20501-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nitrato de nafazolina; Nafazolina, nitrato; Naphazolini nitras

Special notes

When selecting the *Nitrato de nafazolina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nitrato de nafazolina	7	3	27

Second-stage model

For differentiation of the substance/substance group *Nitrato de nafazolina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nitrato de nafazolina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	110,60	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nitrato de nafazolina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nitrato de nafazolina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Nitrato de nafazolina	1512033	22302	60	20160126*
Euro OTC	Nitrato de nafazolina	1810016	24341	40	20181112*
Euro OTC	Nitrato de nafazolina	1910029	24940	40	20191125*
Euro OTC	Nitrato de nafazolina	2004011	25265	40	20200730*
Fagron	Nitrato de nafazolina	12L10-N03	20846	40	20121217
Fagron	Nitrato de nafazolina	12J08-B40-287904	21808	60	20131129
Fagron	Nitrato de nafazolina	22E18-B01-221068	26453	40	20220705

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Nitrato de nafazolina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Nitrato de nafazolina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Nitrato de nafazolina	1512033-01	23275	40
Fagron	Nitrato de nafazolina	16A14-B03-327343	23164	40
Fagron	Nitrato de nafazolina	20D14-F02-370516	25490	40
Fagron	Nitrato de nafazolina	22E18-B01-221068	26453SI†	20

- 201 944 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 42 spectra from 39 *Apo-Ident* customers from 28 batches from the substance/substance group *Nitrato de nafazolina*.

- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Alliance	Nitrato de nafazolina	1810016-02	1
apomix	Nitrato de nafazolina	2004011-01	1
Audor Pharma	Nitrato de nafazolina	12I21-N05	1
Caelo	Nitrato de nafazolina	18K30-B02-357305	1
eurho	Nitrato de nafazolina	2004011-01	1
Euro OTC	Nitrato de nafazolina	1810016-01	1
Euro OTC	Nitrato de nafazolina	191002901	1
Euro OTC	Nitrato de nafazolina	1910029-01	1
Euro OTC	Nitrato de nafazolina	200401101	1
Euro OTC	Nitrato de nafazolina	2004011-01	7
Euro OTC	Nitrato de nafazolina	4011-0001	1
Euro OTC	Nitrato de nafazolina	740530001	1
Euro OTC	Nitrato de nafazolina	740530002	2
Fagron	Nitrato de nafazolina	11I05-N03	1
Fagron	Nitrato de nafazolina	12/21-N05	1
Fagron	Nitrato de nafazolina	12J08-B40	1
Fagron	Nitrato de nafazolina	12J08-B40-287904	1
Fagron	Nitrato de nafazolina	12J08B40-294166	1
Fagron	Nitrato de nafazolina	12J08-B40-294166	1
Fagron	Nitrato de nafazolina	12j08-b40-303401	1
Fagron	Nitrato de nafazolina	140214N	1
Fagron	Nitrato de nafazolina	16A14-B03-322534	1
Fagron	Nitrato de nafazolina	16A14-B03-327343	1
Fagron	Nitrato de nafazolina	16A14-B03-333325	1
Fagron	Nitrato de nafazolina	18K30-B02	1
Fagron	Nitrato de nafazolina	18K30-B02-357305	2
Fagron	Nitrato de nafazolina	20D14-F02-370516	3
Fagron	Nitrato de nafazolina	21021304	1
Fagron	Nitrato de nafazolina	2717M-07042	1
Fagron	Nitrato de nafazolina	740530001	1
Fagron	Nitrato de nafazolina	D14F02-370516	1
Noweda	Nitrato de nafazolina	2004011-03	1

- 236 025 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nitrato de nafazolina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nitrato de nafazolina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	140	0	201 944
Type C	0	40	2	236 025

The substance/substance group *Nitrato de nafazolina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	95.2381 % (> 88.0952 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20846	22302	9,73	231,05
21808	22302	6,68	234,90
22302	22302	0,00	239,34
24341	24341	0,00	240,11
24940	24940	0,00	236,20
25265	25265	0,00	232,01
26453	24940	9,27	238,35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nitrofurantoína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20698-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nitrofurantoína; Nitrofurantoinum

Special notes

When selecting the *Nitrofurantoína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nitrofurantoína	6	3	15

Second-stage model

For differentiation of the substance/substance group *Nitrofurantoína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nitrofurantoína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	140,95	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nitrofurantoína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nitrofurantoína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Nitrofurantoína	12C30-N03	20698	40	1401461
Fagron	Nitrofurantoína	12C30-N03	20837	40	20120417
Fagron	Nitrofurantoína	13B28-N07	21091	40	20130304
Fagron	Nitrofurantoína	15J15-B06-315225	22257	60	AR-16-FG-003763-01
Fagron	Nitrofurantoína	15J15-B06-315225	22322	60	20151028
Fagron	Nitrofurantoína	21J07-B11-219876	26410	40	230502391
Fagron	Nitrofurantoína	21J07-B11-219876	26410SI	20	230502391
Fagron	Nitrofurantoína	22L02-B01-227369	26550	40	20221227
Fagron	Nitrofurantoína	22L02-B01-227369	26550SI	20	20221227
Fagron	Nitrofurantoína	23E23-B06-232014	26901	40	20230630
Fagron	Nitrofurantoína	23E23-B06-232014	26901SI	20	20230630

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 420 spectra of 11 reference samples from the substance/substance group *Nitrofurantoína*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 542 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Nitrofurantoína*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Nitrofurantoína	11K-21-N23	20836	40
Fagron	Nitrofurantoína	11I07-N11	21273	40
Fagron	Nitrofurantoína	23E23-B07-236326	27189	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 28 spectra from 22 *Apo-Ident* customers from 19 batches from the substance/substance group *Nitrofurantoína*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nitrofurantoína	22L02-B01-227369	1
	Nitrofurantoína	22L02-B01-227369	1
Apotheke am Lindenhof	Nitrofurantoína	15J15-B06	1
Fagron	Nitrofurantoína	11/07-N11	1
Fagron	Nitrofurantoína	11F07-N06	3
Fagron	Nitrofurantoína	12C30-N03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Nitrofurantoína	12F19-N02	1
Fagron	Nitrofurantoína	13A08-N01	1
Fagron	Nitrofurantoína	13B28-N07	1
Fagron	Nitrofurantoína	13D10-N03	1
Fagron	Nitrofurantoína	15J15-B06	1
Fagron	Nitrofurantoína	15J15-B06-313939	3
Fagron	Nitrofurantoína	15J15-B06-315225	3
Fagron	Nitrofurantoína	15J15-B06-317250	3
Fagron	Nitrofurantoína	15J15-B06-319031	1
Fagron	Nitrofurantoína	201203080296	1
Fagron	Nitrofurantoína	23E23-B07-236326	1
Fagron	Nitrofurantoína	2714I-03527	1
Fagron	Nitrofurantoína	3071403	1
Fagron	Nitrofurantoína	71/14	1

- 236 039 spectra from 1515 *Apo-Ident* customers from a total of 49 239 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nitrofurantoína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nitrofurantoína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	120	0	201 964
Type C	0	28	0	236 039

The substance/substance group *Nitrofurantoína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 78.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20698	20698	0,00	257,45
20837	20698	5,69	256,86
21091	22257	37,75	230,80
22257	22257	0,00	248,47
22322	22257	4,50	250,10
26410	26410	0,00	286,32
26550	26410	11,90	285,79
26901	26410	12,99	286,09

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ofloxacino**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21047-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ofloxacino; Ofloxacinum

Special notes

When selecting the *Ofloxacino* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ofloxacino	4	2	12

Second-stage model

For differentiation of the substance/substance group *Ofloxacino* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ofloxacino* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato de colamina de cálcio	78,65	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ofloxacino* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ofloxacino*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ofloxacino	13A17-N01	21047	40	1403155
Fagron	Ofloxacino	13A17-N01	21052	40	20130123
Fagron	Ofloxacino	13A17-N01	21811	60	20130123
Fagron	Ofloxacino	15H19-B01-312926	21918	60	20151006
Fagron	Ofloxacino	15H19-B01-325226	23090	40	1707611
Fagron	Ofloxacino	18J30-B01-360431	24598	40	20190419

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Ofloxacino*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 682 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Ofloxacino*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ofloxacino	15H19-B01-337265	23753	40
Fagron	Ofloxacino	22L30-B09-218540	26915	40
Fagron	Ofloxacino	15H19-B01-337265	23754	40
Fagron	Ofloxacino	22L30-B09-218540	26915SI	20

- 201 944 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 12 *Apo-Ident* customers from 13 batches from the substance/substance group *Ofloxacino*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ofloxacino	22L30-B09-218540	1
Caelo	Ofloxacino	15H19-B01	1
Fagron	Ofloxacino	13A17-N01	2
Fagron	Ofloxacino	15H19-B01-314470	1
Fagron	Ofloxacino	15H19-B01-318532	1
Fagron	Ofloxacino	15H19-B01-337265	1
Fagron	Ofloxacino	15H1-OF-M20150401B	1
Fagron	Ofloxacino	18J30-B01	2
Fagron	Ofloxacino	18J30-B01_363954	1
Fagron	Ofloxacino	18J30-B01-363954	3
Fagron	Ofloxacino	B01-3619609	1
Fagron	Ofloxacino	B01-3639504	1
Fragon	Ofloxacino	15H19-B01-343412	1

- 236 050 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ofloxacino* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ofloxacino* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	140	0	201 944
Type C	0	17	0	236 050

The substance/substance group *Ofloxacino* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21047	21047	0,00	166,03
21052	21047	6,97	165,19
21811	23090	18,89	146,58
21918	23090	16,18	148,02
23090	23090	0,00	166,84
24598	23090	10,09	171,07

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Omeprazol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21098-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Omeprazol; Omeprazolum

Special notes

When selecting the *Omeprazol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Omeprazol	6	3	130

Second-stage model

For differentiation of the substance/substance group *Omeprazol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Omeprazol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Acetato de ciproterona	96,43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Omeprazol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Omeprazol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Omeprazol	15K12-B02-314608	22740	40	20151124
Fagron	Omeprazol	15K12-B02-314608	22890	40	20151124
Fagron	Omeprazol	19F14-B01-362735	24768	40	1910227
Fagron	Omeprazol	20F18-F21-375443	25582	40	20200715
Fagron	Omeprazol	22G08-B01-221106	26384	40	20220714
Fagron	Omeprazol	22L08-B02-225402	26539	40	20221228
Inresa	Omeprazol	OPFP14017	21787	60	1507407
Inresa	Omeprazol	OPFP14017	21796	60	20140228
Inresa	Omeprazol	OPFP14017	22284	60	20140528
Inresa	Omeprazol	OPFP14017	23273	40	20150428

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Omeprazol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

different batches.

- 152 502 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Omeprazol*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Omeprazol	16I20-B03-328940	23272	40
Fagron	Omeprazol	18K01-B03-358185	24583	40
Fagron	Omeprazol	22C31-B01-218818	26151	40
Fagron	Omeprazol	22C31-B01-218818	26151SI	20
Fagron	Omeprazol	22G08-B01-221106	26384SI†	20
Fagron	Omeprazol	22L08-B02-225402	26539SI†	20

- 201 904 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 534 spectra from 192 *Apo-Ident* customers from 145 batches from the substance/substance group *Omeprazol*.

- Among them are spectra of independent samples from 130 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Omeprazol		1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Omeprazol	20F18-F21-371963	1
	Omeprazol	21D08-F03-526980	1
	Omeprazol	22C31-B01-218818	3
	Omeprazol	22G08-B01-221106	1
	Omeprazol	22G-08-B01-221106	1
	Omeprazol	22L08-B02-225402	15
	Omeprazol	22L08-B02-225421	1
	Omeprazol	23C16-B08-227714	1
	Omeprazol	23C16-B08-230403	1
	Omeprazol	23C16-B08-230663	1
	Omeprazol	23G31-B06-232416	2
	Omeprazol	23H09-B05-234459	1
	Omeprazol	B06-2324106	1
	Omeprazol	B08-2346505	1
	Omeprazol	OPFP21008	1
	Omeprazol	OPFP21028	2
	Omeprazol	OZ23010	1
agron/Noweda	Omeprazol	18K01B03358185	2
AHD	Omeprazol	22L08-B02-225402	4
Alliance Healthcare	Omeprazol	20F18-F21-375443	1
Caelo	Omeprazol	15k12b022314608	1
Caelo	Omeprazol	15K12B02314608	1
Caelo	Omeprazol	16l20-B03-329040	1
Caelo	Omeprazol	17H15-B03	1
Caelo	Omeprazol	17H15-B03-340200	2
Caelo	Omeprazol	17H15-B03342821	1
Caelo	Omeprazol	17K28-B07-348698	6
Caelo	Omeprazol	18E22-B03-353496	1
Caelo	Omeprazol	18K01-B03-358185	1
Caelo	Omeprazol	19F14-B01	1
Caelo	Omeprazol	20f18-f21-371963	1
Caelo	Omeprazol	21D08-F03-526829	1
Caelo	Omeprazol	22444	2
Fagron	Omeprazol		1
Fagron	Omeprazol	15B26-B40-305669	2
Fagron	Omeprazol	15k12-B02	1
Fagron	Omeprazol	15K12-B02	2
Fagron	Omeprazol	15K12-B02-314608	7
Fagron	Omeprazol	15K12-B02-525174	2
Fagron	Omeprazol	16/20-B03	1
Fagron	Omeprazol	16/20-B03-328940	4
Fagron	Omeprazol	16B16-B01-52535	1
Fagron	Omeprazol	16I20-B03-328940	7
Fagron	Omeprazol	16J20-B03-328940	1
Fagron	Omeprazol	16l20-B03-328940	1
Fagron	Omeprazol	17B28-B02	2
Fagron	Omeprazol	17B28-B02-525511	2
Fagron	Omeprazol	17-B28-B02-525511	1
Fagron	Omeprazol	17B28-B02-525557	3
Fagron	Omeprazol	17H15-B03	2
Fagron	Omeprazol	17H15-B03-340200	1
Fagron	Omeprazol	17h15-b03-342821	1
Fagron	Omeprazol	17H15B03342821	1
Fagron	Omeprazol	17H15-B03-342821	18
Fagron	Omeprazol	17h15b0334821	1
Fagron	Omeprazol	17K28-B07	2
Fagron	Omeprazol	17k28b07348698	1
Fagron	Omeprazol	17K28-B07-348698	16
Fagron	Omeprazol	17K28-B07-3486998	1
Fagron	Omeprazol	18E22-B03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Omeprazol	18e22b03353496	1
Fagron	Omeprazol	18E22B03353496	1
Fagron	Omeprazol	18E22-B03-353496	12
Fagron	Omeprazol	18e22-b03-353496	1
Fagron	Omeprazol	18K01-B03	2
Fagron	Omeprazol	18K01-B03-358185	16
Fagron	Omeprazol	18K01-B03-358186	2
Fagron	Omeprazol	19F14	1
Fagron	Omeprazol	19F14-B01	4
Fagron	Omeprazol	19F14-B01-362735	14
Fagron	Omeprazol	19f14-B01-363425	1
Fagron	Omeprazol	19F14B01363425	1
Fagron	Omeprazol	19F14-B01-363425	14
Fagron	Omeprazol	19F14-B01-363427	1
Fagron	Omeprazol	19F14-B01-36345	2
Fagron	Omeprazol	19F14-B01-526150	4
Fagron	Omeprazol	19F14B01526150Set19L06-Ko2	1
Fagron	Omeprazol	19F-B01-363425	1
Fagron	Omeprazol	19J29-F03	2
Fagron	Omeprazol	19J29-F03-367825	12
Fagron	Omeprazol	19L09-K02	1
Fagron	Omeprazol	20A16-F02	6
Fagron	Omeprazol	20A16-F02-367834	3
Fagron	Omeprazol	20A16-F02-368827	9
Fagron	Omeprazol	20A16-F02-368828	2
Fagron	Omeprazol	20A16-F02-368827	1
Fagron	Omeprazol	20A416-F02-368827	1
Fagron	Omeprazol	20F18-F21	5
Fagron	Omeprazol	20F18-F21-371963	24
Fagron	Omeprazol	20F18-F21-3754403	1
Fagron	Omeprazol	20F18F21375443	1
Fagron	Omeprazol	20F18-F21-375443	32
Fagron	Omeprazol	20F18-F21-526401	2
Fagron	Omeprazol	20J27-F02	2
Fagron	Omeprazol	20J27-F02-376140	1
Fagron	Omeprazol	20j27-f02-526599	1
Fagron	Omeprazol	20J27-F02-526599	3
Fagron	Omeprazol	20J27F-F02-376140	1
Fagron	Omeprazol	21/01-B05-213885	1
Fagron	Omeprazol	21101-B05-213885	1
Fagron	Omeprazol	21101-BO5-213885	2
Fagron	Omeprazol	21C30-B03	1
Fagron	Omeprazol	21C30-B03-215335	1
Fagron	Omeprazol	21D08F03526829	1
Fagron	Omeprazol	21D08-F03-526829	2
Fagron	Omeprazol	21D08-F03-526980	1
Fagron	Omeprazol	21H04-B12-213937	2
Fagron	Omeprazol	21I01-B05	3
Fagron	Omeprazol	21I01-B05_213885	1
Fagron	Omeprazol	21I01-B05-213885	32
Fagron	Omeprazol	21I01-B05-217276	3
Fagron	Omeprazol	21I1-B05	1
Fagron	Omeprazol	21l01-B05-21028	1
Fagron	Omeprazol	21l01-B05-213885	4
Fagron	Omeprazol	21O01-B05-213885	1
Fagron	Omeprazol	22C31-B01	1
Fagron	Omeprazol	22C31-B01-218672	2
Fagron	Omeprazol	22c31-b01-218818	1
Fagron	Omeprazol	22C31B01218818	1
Fagron	Omeprazol	22C31B-01-218818	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Omeprazol	22C31-B01-218818	21
Fagron	Omeprazol	22C31-B01-21888	1
Fagron	Omeprazol	22C31-BO1-218818	2
Fagron	Omeprazol	22G08-B01	1
Fagron	Omeprazol	22G08-B01-221106	16
Fagron	Omeprazol	22L08-B02_225402	1
Fagron	Omeprazol	22L08-B02-225402	8
Fagron	Omeprazol	22LO8-BO2-2225402	1
Fagron	Omeprazol	20F18-F21-371963	1
Fagron	Omeprazol	20F18-F21-375443	1
Fagron	Omeprazol	70192525	1
Fagron	Omeprazol	73590-58-6	1
Fagron	Omeprazol	b01-2188108	1
Fagron	Omeprazol	B01-3634205	2
Fagron	Omeprazol	B01-526150	2
Fagron	Omeprazol	B05-2138805	3
Fagron	Omeprazol	B05-213885	1
Fagron	Omeprazol	F02-3678304	2
Fagron	Omeprazol	F02-3688207	1
Fagron	Omeprazol	F02-3761400	1
Fagron	Omeprazol	F03-3678205	5
Fagron	Omeprazol	F03-5268209	1
Fagron	Omeprazol	F21-3719603	3
Fagron	Omeprazol	F21-3719605	1
Fagron	Omeprazol	F21-3754403	1
Fagron	Omeprazol	OPFP16030	1
Fagron	Omeprazol	OPFP17033	3
Fagron	Omeprazol	OPFP18052	2
Fagron	Omeprazol	OPFP18052/18K01-B03-358185	1
Fagron	Omeprazol	OPFP19002	3
Fagron	Omeprazol	OPFP19002/19F14-B01-526150	1
Fagron	Omeprazol	OPFP19017	1
Fagron	Omeprazol	OPFP20024	7
Fagron	Omeprazol	OPFP21028	3
Fargon/AHD	Omeprazol	17K28-B07	1
Fargon/AHD	Omeprazol	18K01-B03	1
Fargon/Fiebig	Omeprazol	18K01-B03	1
Fargon/Phönix	Omeprazol	21I01-B05-213885	1
Fargon	Omeprazol	19J29-F03-367825	1
Ferdinand Eimermacher	Omeprazol	4271019	1
Fragon	Omeprazol	17K28-B07-348698	1
Gehe	Omeprazol	17H15-B03-342821	1
Lee Pharma Limited/ Gehe	Omeprazol	19F14-B01-363425	2
Lee Pharma Ltd.	Omeprazol	21101-B05-213885	1
Noveda	Omeprazol	21D08-F03-526980	1
Noweda	Omeprazol	15K15-B02-314608	1
Noweda	Omeprazol	17H15-B03-342821	3
noweda	Omeprazol	19j29-f03-367825	1
Noweda	Omeprazol	22G08-B01-221106	1
Noweda	Omeprazol	22L08-B02-225402	1
Phoenix	Omeprazol	18E22-B03-353496	4
Phönix	Omeprazol	17K28-B07-348698	2
Phönix	Omeprazol	20A16-F02-368827	1
Phönix	Omeprazol	21I01B05213885	1
Phönix	Omeprazol	22C31-B01-218818	4
Sanacorp	Omeprazol	17H15-B03-342821	1
SANACORP	Omeprazol	21I01-B05-213885	1
Sanacorp	Omeprazol	22L08B02225402	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 533 spectra from 1515 *Apo-Ident* customers from a total of 49 113 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Omeprazol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Omeprazol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	180	0	201 904
Type C	0	514	20	235 533

The substance/substance group *Omeprazol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	96.2547 % (> 95.6929 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21787	21787	0,00	96,58
21796	21787	4,75	98,11
22284	21787	4,60	95,45
22740	21787	15,19	93,30
22890	21787	14,90	97,33
23273	21787	6,96	100,77
24768	24768	0,00	121,93
25582	21787	7,65	101,83
26384	21787	5,72	96,08
26539	21787	5,48	96,64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Orlistate**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006683-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Orlistate

Special notes

When selecting the *Orlistate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Orlistate	2	2	0

Second-stage model

For differentiation of the substance/substance group *Orlistate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Orlistate* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Valerato de estradiol	123,29	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Orlistate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Orlistate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Orlistate	6012307004-01	BR20020	40	20240523*
Fagron	Orlistate	6012307003-02	BR20023	40	20240526*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Orlistate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 6 reference samples from the substance/substance group *Orlistate*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Orlistate	2406002	BR20024	40
Fagron	Orlistate	6012307007-01	BR20025	40
Fagron	Orlistate	6012307004-01	BR20020SI†	20
Fagron	Orlistate	6012307003-02	BR20023SI†	20
Fagron	Orlistate	2406002	BR20024SI	20
Fagron	Orlistate	6012307007-01	BR20025SI	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Orlistate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Orlistate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Orlistate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	160	0	201 924
Type C	0	0	0	236 067

The substance/substance group *Orlistate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
BR20020	BR20020	0,00	136,07
BR20023	BR20023	0,00	134,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Orotato de lítio monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21055-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Orotato de lítio monoidratado; Lithii orotas monohydricum

Special notes

When selecting the *Orotato de lítio monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Orotato de lítio monoidratado	9	9	4

Second-stage model

For differentiation of the substance/substance group *Orotato de lítio monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Orotato de lítio monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	98,43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Orotato de lítio monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Orotato de lítio monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Orotato de lítio monoidratado	2009002	25404	40	20201020*
Euro OTC	Orotato de lítio monoidratado	2102007	25523	40	20210222*
Euro OTC	Orotato de lítio monoidratado	2210011	26431	40	20221107*
Euro OTC	Orotato de lítio monoidratado	2210011	26431SI	20	20221107*
Euro OTC	Orotato de lítio monoidratado	2403013	27207	40	20240508*
Fagron	Orotato de lítio monoidratado	13J04-N01	21055	40	1405616
Fagron	Orotato de lítio monoidratado	13I09-B04-290311	21688	60	20130927
Fagron	Orotato de lítio monoidratado	15F25-B01-315219	22502	40	20150716
Fagron	Orotato de lítio monoidratado	18K21-B01-363417	25063	40	20181231
Fagron	Orotato de lítio monoidratado	22B26-B12-227899	26541	40	20220608
Fagron	Orotato de lítio monoidratado	22B26-B12-227899	26541SI	20	20220608

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 11 reference samples from the substance/substance group *Orotato de lítio monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 10 reference samples from the substance/substance group *Orotato de lítio monoidratado*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Orotato de lítio monoidratado	2002030	25146	40
Euro OTC	Orotato de lítio monoidratado	2110013	25882	50
Euro OTC	Orotato de lítio monoidratado	2311026	26994	40
Euro OTC	Orotato de lítio monoidratado	2311003	26995	40
Euro OTC	Orotato de lítio monoidratado	2407006	27351	40
Euro OTC	Orotato de lítio monoidratado	2408005	27352	40
Euro OTC	Orotato de lítio monoidratado	2408006	27353	40
Fagron	Orotato de lítio monoidratado	16D15-B08-321402	23269	40
Fagron	Orotato de lítio monoidratado	18A19-B12-347442	24111	40
Euro OTC	Orotato de lítio monoidratado	2110013	25882SI	10

- 201 704 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Orotato de lítio monoidratado*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Orotato de lítio monoidratado	23K07-B10-232375	1
	Orotato de lítio monoidratado	2408005-01	2
AHD	Orotato de lítio monoidratado	2407006-01	1
Euro OTC	Orotato de lítio monoidratado	2408005-01	1
Fagron	Orotato de lítio monoidratado	13J04-N01	1
Pfannenschmidt	Orotato de lítio monoidratado	ORL00212	1

- 236 060 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Orotato de lítio monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Orotato de lítio monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	380	0	201 704
Type C	0	7	0	236 060

The substance/substance group *Orotato de lítio monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21055	21055	0,00	193,11
21688	21055	5,84	190,86
22502	21055	8,71	192,10
25063	25523	5,49	191,42
25404	25404	0,00	188,12
25523	25523	0,00	189,03
26431	26431	0,00	193,20
26541	25404	6,43	190,46
27207	27207	0,00	188,65

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Orotato de magnésio di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20429-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Orotato de magnésio di-hidratado; Magnesii orotas dihydricus

Special notes

When selecting the *Orotato de magnésio di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Orotato de magnésio di-hidratado	7	17	36

Second-stage model

For differentiation of the substance/substance group *Orotato de magnésio di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Orotato de magnésio di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Orotato de manganês di-hidratado	76,61	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Orotato de magnésio di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Orotato de magnésio di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Orotato de magnésio di-hi…	162227	22638	40	20160809*
Caelo	Orotato de magnésio di-hi…	16222701	23236	40	20160809
Euro OTC	Orotato de magnésio di-hi…	1511021	22287	60	20151228*
Euro OTC	Orotato de magnésio di-hi…	1707018	23615	40	20170907*
Euro OTC	Orotato de magnésio di-hi…	1911024	25069	40	20200107*
Euro OTC	Orotato de magnésio di-hi…	2003014	25147	40	20200416*
Euro OTC	Orotato de magnésio di-hi…	2309021	26926	40	20231011*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Orotato de magnésio di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 750 spectra of 21 reference samples from the substance/substance group *Orotato de magnésio di-hidratado*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Orotato de magnésio di-hi…	172157	23661	40
Caelo	Orotato de magnésio di-hi…	172547	23799	40
Euro OTC	Orotato de magnésio di-hi…	1608017	22784	40
Euro OTC	Orotato de magnésio di-hi…	1712001	23874	40
Euro OTC	Orotato de magnésio di-hi…	1802018	23963	40
Euro OTC	Orotato de magnésio di-hi…	1808029	24200	40
Euro OTC	Orotato de magnésio di-hi…	1902007	24490	40
Euro OTC	Orotato de magnésio di-hi…	1906014	24797	40
Euro OTC	Orotato de magnésio di-hi…	1909007	24835	40
Euro OTC	Orotato de magnésio di-hi…	2006004	25341	40
Euro OTC	Orotato de magnésio di-hi…	2102003	25595	40
Euro OTC	Orotato de magnésio di-hi…	2109023	25892	50
Euro OTC	Orotato de magnésio di-hi…	2202010	25969	40
Euro OTC	Orotato de magnésio di-hi…	2207009	26196	40
Euro OTC	Orotato de magnésio di-hi…	2301041	26584	40
Euro OTC	Orotato de magnésio di-hi…	2403014	27214	40
Euro OTC	Orotato de magnésio di-hi…	2408014	27399	40
Euro OTC	Orotato de magnésio di-hi…	2109023	25892SI	10
Euro OTC	Orotato de magnésio di-hi…	2202010	25969SI	10
Euro OTC	Orotato de magnésio di-hi…	2207009	26196SI	20
Euro OTC	Orotato de magnésio di-hi…	2301041	26584SI	20

- 201 334 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 62 spectra from 25 *Apo-Ident* customers from 36 batches from the substance/substance group *Orotato de magnésio di-hidratado*.
- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Orotato de magnésio di-hi…	14093607	2
Caelo	Orotato de magnésio di-hi…	1808029-01	1
EuRho	Orotato de magnésio di-hi…	2102003-01	1
Euro OTC	Orotato de magnésio di-hi…	1209029-01	3
Euro OTC	Orotato de magnésio di-hi…	1305011-01	1
Euro OTC	Orotato de magnésio di-hi…	130501102	1
Euro OTC	Orotato de magnésio di-hi…	1305011-02	5
Euro OTC	Orotato de magnésio di-hi…	1407005-01	3
Euro OTC	Orotato de magnésio di-hi…	1504002-01	1
Euro OTC	Orotato de magnésio di-hi…	1504002-02	1
Euro OTC	Orotato de magnésio di-hi…	151102101	1
Euro OTC	Orotato de magnésio di-hi…	1511021-02	6
Euro OTC	Orotato de magnésio di-hi…	1608017-01	2
Euro OTC	Orotato de magnésio di-hi…	1608017-02	1
Euro OTC	Orotato de magnésio di-hi…	16085017-01	1
Euro OTC	Orotato de magnésio di-hi…	1707018-01	4
Euro OTC	Orotato de magnésio di-hi…	1712001-01	2
Euro OTC	Orotato de magnésio di-hi…	1802018-01	1
Euro OTC	Orotato de magnésio di-hi…	1808029-01	1
Euro OTC	Orotato de magnésio di-hi…	180802902	1
Euro OTC	Orotato de magnésio di-hi…	1906014-01	2
Euro OTC	Orotato de magnésio di-hi…	1909007-01	2
Euro OTC	Orotato de magnésio di-hi…	2003014-01	2
Euro OTC	Orotato de magnésio di-hi…	2006004-01	1
Euro OTC	Orotato de magnésio di-hi…	2102003-01	1
Euro OTC	Orotato de magnésio di-hi…	2109023-01	3
Euro OTC	Orotato de magnésio di-hi…	2109023-02	1
Fagron	Orotato de magnésio di-hi…	1000060461	1
Fagron	Orotato de magnésio di-hi…	12G05-N03	1
Fagron	Orotato de magnésio di-hi…	13H06-N07	1
Fagron	Orotato de magnésio di-hi…	14/13-B05-305616	1
Fagron	Orotato de magnésio di-hi…	14E20-B05-296005	1
Fagron	Orotato de magnésio di-hi…	160801701	1
Fagron	Orotato de magnésio di-hi…	16K22B01329783	1
Fagron	Orotato de magnésio di-hi…	17H14-B02	1
Fagron	Orotato de magnésio di-hi…	17H14B02346538	1
Fagron	Orotato de magnésio di-hi…	354317	1
Noweda	Orotato de magnésio di-hi…	2301041-01	1

- 236 005 spectra from 1515 *Apo-Ident* customers from a total of 49 223 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Orotato de magnésio di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Orotato de magnésio di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	750	0	201 334
Type C	0	62	0	236 005

The substance/substance group *Orotato de magnésio di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.3226 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22287	22287	0,00	139,36
22638	22638	0,00	153,66
23236	22638	7,68	154,31
23615	23615	0,00	142,22
25069	25069	0,00	151,51
25147	25147	0,00	150,78
26926	26926	0,00	143,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Orotato de manganês di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22311-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Orotato de manganês di-hidratado

Special notes

When selecting the *Orotato de manganês di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Orotato de manganês di-hidratado	5	2	1

Second-stage model

For differentiation of the substance/substance group *Orotato de manganês di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Orotato de manganês di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Orotato de magnésio di-hidratado	83,14	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Orotato de manganês di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Orotato de manganês di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Orotato de manganês di-hi…	1601003	22311	60	20160113*
Euro OTC	Orotato de manganês di-hi…	1801031	23908	40	20180131*
Euro OTC	Orotato de manganês di-hi…	1907009	24787	40	20190718*
Euro OTC	Orotato de manganês di-hi…	2208027	26265	40	20220905*
Euro OTC	Orotato de manganês di-hi…	2311027	27073	40	20231221*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Orotato de manganês di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 742 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Orotato de manganês di-hidratado*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Orotato de manganês di-hi…	1605029-01	22654	40
Euro OTC	Orotato de manganês di-hi…	2010007	25466	40
Euro OTC	Orotato de manganês di-hi…	1605029-01	22737	40
Euro OTC	Orotato de manganês di-hi…	2208027	26265SI†	20
Euro OTC	Orotato de manganês di-hi…	2311027	27073SI†	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Orotato de manganês di-hidratado*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Orotato de manganês di-hi…	1907009-02	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Orotato de manganês di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Orotato de manganês di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	160	0	201 924
Type C	0	1	0	236 066

The substance/substance group *Orotato de manganês di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22311	22311	0,00	163,70
23908	23908	0,00	146,77
24787	24787	0,00	145,40
26265	26265	0,00	162,33
27073	27073	0,00	165,96

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Orotato de zinco di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20424-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Orotato de zinco di-hidratado; Zincum oroticum dihydricum

Special notes

When selecting the *Orotato de zinco di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Orotato de zinco di-hidratado	3	1	1

Second-stage model

For differentiation of the substance/substance group *Orotato de zinco di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Orotato de zinco di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloreto de alumínio hexa-hidratado	86,40	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Orotato de zinco di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Orotato de zinco di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Orotato de zinco di-hidratado	1203014-01	21038	40	1407431
Euro OTC	Orotato de zinco di-hidratado	13050005-02	21326	40	20130628*
Euro OTC	Orotato de zinco di-hidratado	2312002	26993	40	20231214*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Orotato de zinco di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 842 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Orotato de zinco di-hidratado*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Orotato de zinco di-hidratado	2302021	26631	40
Euro OTC	Orotato de zinco di-hidratado	2302021	26631SI	20
Euro OTC	Orotato de zinco di-hidratado	2312002	26993SI†	20

- 202 004 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Orotato de zinco di-hidratado*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Ichtyol/Phönix	Orotato de zinco di-hidratado	12B02-N02	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Orotato de zinco di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Orotato de zinco di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	80	0	202 004
Type C	0	0	1	236 066

The substance/substance group *Orotato de zinco di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21038	21038	0,00	231,09
21326	21326	0,00	238,47
26993	26993	0,00	152,27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Oxetacaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	23686-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxetacaína; Oxetacainum

Special notes

When selecting the *Oxetacaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Oxetacaína	5	1	20

Second-stage model

For differentiation of the substance/substance group *Oxetacaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oxetacaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Propionato de clobetasol	109,99	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Oxetacaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Oxetacaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Oxetacaína	AP010-160120	24104	40	1809415
Caelo	Oxetacaína	172498	23686	40	20170925*
Caelo	Oxetacaína	191134	24757	40	20190523*
Euro OTC	Oxetacaína	2002021	25254	40	20200612*
Euro OTC	Oxetacaína	2002020-01	25293	40	20200714

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Oxetacaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 50 spectra of 1 reference samples from the substance/substance group *Oxetacaína*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxetacaína	17249805	23916	50

- 202 034 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 87 spectra from 67 *Apo-Ident* customers from 20 batches from the substance/substance group *Oxetacaína*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Oxetacaína	2002020-03	1
	Oxetacaína	2002020-13	1
	Oxetacaína	21001626004	1
	Oxetacaína	21001626006	5
	Oxetacaína	21001626008	1
Caelo	Oxetacaína	17249805	1
Caelo	Oxetacaína	17249806	1
Caelo	Oxetacaína	17249808	1
Caelo	Oxetacaína	17249809	1
Caelo	Oxetacaína	17249810	6
Caelo	Oxetacaína	191134001	7
Caelo	Oxetacaína	191134002	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Oxetacaína	191134005	5
Caelo	Oxetacaína	191134007	5
Caelo	Oxetacaína	19113401	8
Caelo	Oxetacaína	19113402	9
Caelo	Oxetacaína	21001626002	3
Caelo	Oxetacaína	21001626004	1
Caelo	Oxetacaína	91134002	1
Caesar & Loretz GmbH…	Oxetacaína	191134007	1
Caesar & Loretz GmbH…	Oxetacaína	191134005	1
Caesar & Loretz GmbH…	Oxetacaína	191134007	1
Caesar & Loretz GmbH…	Oxetacaína	19113402	1
Caesar & Loretz GmbH…	Oxetacaína	191134002	2
Caesar & Loretz GmbH	Oxetacaína	191134001	4
CAESAR & LORETZ GMBH	Oxetacaína	191134002	1
Caesar & Loretz GmbH	Oxetacaína	191134005	1
Caesar & Loretz GmbH	Oxetacaína	191134007	2
Caesar&Lorenz	Oxetacaína	191134005	1
EuRho	Oxetacaína	2002021-01	1
Euro OTC	Oxetacaína	2002020-02	1
Euro OTC	Oxetacaína	2002020-03	3
Euro OTC	Oxetacaína	2002021-01	1
Kehr	Oxetacaína	17249805	1

- 235 980 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Oxetacaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxetacaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	50	0	202 034
Type C	0	87	0	235 980

The substance/substance group *Oxetacaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 88.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.1034 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23686	23686	0,00	141,70
24104	24104	0,00	147,33
24757	24757	0,00	142,54
25254	25254	0,00	149,69
25293	24104	10,03	145,37

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Palmitato de ascorbila**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21053-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Palmitato de ascorbila; Ascorbylis palmitas

Special notes

When selecting the *Palmitato de ascorbila* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Palmitato de ascorbila	7	5	213

Second-stage model

For differentiation of the substance/substance group *Palmitato de ascorbila* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Palmitato de ascorbila* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estriol	85,47	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Palmitato de ascorbila* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Palmitato de ascorbila*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Palmitato de ascorbila	13K04-N01	21053	40	1403226
Fagron	Palmitato de ascorbila	13C06-B40-291206	21665	60	20140306
Fagron	Palmitato de ascorbila	15F01-B99-309774	21851	60	20150615
Fagron	Palmitato de ascorbila	17E18-B06-335527	23520	40	20170606
Fagron	Palmitato de ascorbila	17E18-B06-335527	23520SI	40	20170606
Fagron	Palmitato de ascorbila	19D25-B04-361254	24665	40	20190517
Fagron	Palmitato de ascorbila	20L07-F01-375723	25583	40	20201223
Fagron	Palmitato de ascorbila	20L07-F01-375723	25583SI	40	20201223
Fagron	Palmitato de ascorbila	24I26-B11-004333	27471	40	20241007
Fagron	Palmitato de ascorbila	24I26-B11-004333	27471SI	40	20241007

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Palmitato de ascorbila*. These samples are listed above in the *calibration samples* section. The reference samples come

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 11 reference samples from the substance/substance group *Palmitato de ascorbila*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Palmitato de ascorbila	17H04-B01-338484	23987	40
Fagron	Palmitato de ascorbila	18A10-B03-344364	24098	40
Fagron	Palmitato de ascorbila	21G17-B04-213672	26058	40
Fagron	Palmitato de ascorbila	22F07-B01-222885	26604	40
Fagron	Palmitato de ascorbila	23A09-B04-228316	26605	40
Fagron	Palmitato de ascorbila	17H04-B01-338484	23987SI	40
Fagron	Palmitato de ascorbila	18A10-B03-344364	24098SI	40
Fagron	Palmitato de ascorbila	19D25-B04-361254	24665SI†	40
Fagron	Palmitato de ascorbila	21G17-B04-213672	26058SI	40
Fagron	Palmitato de ascorbila	22F07-B01-222885	26604SI	40
Fagron	Palmitato de ascorbila	23A09-B04-228316	26605SI	40

- 201 644 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 698 spectra from 335 *Apo-Ident* customers from 231 batches from the substance/substance group *Palmitato de ascorbila*.

- Among them are spectra of independent samples from 212 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Palmitato de ascorbila	18B12-B09-525889	1
	Palmitato de ascorbila	21G17-B04-213672	1
	Palmitato de ascorbila	21L16-B09-217351	1
	Palmitato de ascorbila	21L16-B09-221849	1
	Palmitato de ascorbila	22F07-B01	1
	Palmitato de ascorbila	22F07-B01-222885	10
	Palmitato de ascorbila	23A09-B04-228316	6
	Palmitato de ascorbila	23Ao9-B04-228316	1
18J22-B03-525911	Palmitato de ascorbila	Fagron	1
AHC	Palmitato de ascorbila	23A09-B04-228316	1
AHD	Palmitato de ascorbila	23A09-B04-228316	1
Bionorica Ethics/ Noweda	Palmitato de ascorbila	85532	2
Bionorica Ethics	Palmitato de ascorbila	82275	1
Bionorica ethics	Palmitato de ascorbila	85532	2
Bionorica Ethics7Noweda	Palmitato de ascorbila	82275	2
Bionorica EthicsGmbH...	Palmitato de ascorbila	74736	1
Bionorica/Noweda	Palmitato de ascorbila	82275	1
Bionorica/Noweda	Palmitato de ascorbila	85532	2
Bionorica	Palmitato de ascorbila	74736	1
Bionorica	Palmitato de ascorbila	74962	1
Bionorica	Palmitato de ascorbila	82275	1
Bionorica	Palmitato de ascorbila	85532	1
Bombastus	Palmitato de ascorbila	525526	1
Caelo	Palmitato de ascorbila	15F01-B99-525121	1
Caelo	Palmitato de ascorbila	16810-B04525199	1
Caelo	Palmitato de ascorbila	16B10-B04324111	1
Caelo	Palmitato de ascorbila	16B10-B04-525199	1
Caelo	Palmitato de ascorbila	16B-B04-525283	1
Caelo	Palmitato de ascorbila	16I30-B03-525489	1
Caelo	Palmitato de ascorbila	16l30-B03-525358	2
Caelo	Palmitato de ascorbila	17E18-B06	1
Caelo	Palmitato de ascorbila	17E18-B06-334914	1
Caelo	Palmitato de ascorbila	17H04-B01-525632	1
Caelo	Palmitato de ascorbila	18A10-B03	1
Caelo	Palmitato de ascorbila	18A10-B03-344364	2
Caelo	Palmitato de ascorbila	18B12-B09-525720	1
Caelo	Palmitato de ascorbila	18B12-B09-525721	1
Caelo	Palmitato de ascorbila	18J22-B03-355582	1
Caelo	Palmitato de ascorbila	19D25-B04-361254	2
Caelo	Palmitato de ascorbila	20I01-F04-52693	1
Caelo	Palmitato de ascorbila	B04-2136007	1
Caelo	Palmitato de ascorbila	K50264890	1
DSM Nutritional GmbH	Palmitato de ascorbila	20L07-F01-526513	1
Euro OTC	Palmitato de ascorbila	16I30-B03	1
Euro OTC	Palmitato de ascorbila	17H04-B0152632	1
Euro OTC	Palmitato de ascorbila	77773	2
Fagrin/Noweda	Palmitato de ascorbila	18B12-B09525720	1
Fagron	Palmitato de ascorbila		7
Fagron	Palmitato de ascorbila	10061708	1
Fagron	Palmitato de ascorbila	137-66-6	2
Fagron	Palmitato de ascorbila	13C06-B40-291206	2
Fagron	Palmitato de ascorbila	14I03-N01	1
Fagron	Palmitato de ascorbila	15F01-B99	3
Fagron	Palmitato de ascorbila	15f01-b99-309774	1
Fagron	Palmitato de ascorbila	15F01-B99-52063	1
Fagron	Palmitato de ascorbila	15F01-B99-525063	1
Fagron	Palmitato de ascorbila	15F01-B99-525121	1
Fagron	Palmitato de ascorbila	15F01-B99-525122	2
Fagron	Palmitato de ascorbila	16/30-B03	1
Fagron	Palmitato de ascorbila	16/30-B03-329375	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Palmitato de ascorbila	16/30-B03-330625	3
Fagron	Palmitato de ascorbila	1630-B03-525489	1
Fagron	Palmitato de ascorbila	16B10-B04-525199	2
Fagron	Palmitato de ascorbila	16B10-B04-525228	1
Fagron	Palmitato de ascorbila	16B10-B04-525283	1
Fagron	Palmitato de ascorbila	16I30-B03	3
Fagron	Palmitato de ascorbila	16I30-B03-326543	1
Fagron	Palmitato de ascorbila	16I30-B03-329375	1
Fagron	Palmitato de ascorbila	16I30-B03-330625	1
Fagron	Palmitato de ascorbila	16I30-B03-332623	5
Fagron	Palmitato de ascorbila	16I30-B03-525358	3
Fagron	Palmitato de ascorbila	16I30-B03-525380	2
Fagron	Palmitato de ascorbila	16I30-B03-525425	1
Fagron	Palmitato de ascorbila	16I30-B03-525426	1
Fagron	Palmitato de ascorbila	16I30-B03-525489	1
Fagron	Palmitato de ascorbila	16L30-B03-332623	1
Fagron	Palmitato de ascorbila	17e18-b06	2
Fagron	Palmitato de ascorbila	17E18-B06	1
Fagron	Palmitato de ascorbila	17e18b06334914	1
Fagron	Palmitato de ascorbila	17E18-B06-334914	2
Fagron	Palmitato de ascorbila	17E18-B06-335527	3
Fagron	Palmitato de ascorbila	17E18-B06-336731	2
Fagron	Palmitato de ascorbila	17E18-B06-525514	1
Fagron	Palmitato de ascorbila	17E18-B06-5255225	1
Fagron	Palmitato de ascorbila	17E18-B06-525524	4
Fagron	Palmitato de ascorbila	17E18-B06-525525	1
Fagron	Palmitato de ascorbila	17E18-B06-525526	2
Fagron	Palmitato de ascorbila	17H04-B01	1
Fagron	Palmitato de ascorbila	17H04B01338484	1
Fagron	Palmitato de ascorbila	17H04-B01-338484	8
Fagron	Palmitato de ascorbila	17H04B01340474	2
Fagron	Palmitato de ascorbila	17H04-B01-340474	3
Fagron	Palmitato de ascorbila	17h04-b01-525632	1
Fagron	Palmitato de ascorbila	17H04-B01-525632	4
Fagron	Palmitato de ascorbila	18812b09348867	1
Fagron	Palmitato de ascorbila	18812-B09-525719	2
Fagron	Palmitato de ascorbila	18812-B09-525720	3
Fagron	Palmitato de ascorbila	18812-B09-525721	1
Fagron	Palmitato de ascorbila	188B12-B09-525721	1
Fagron	Palmitato de ascorbila	18A10_B03_344364	1
Fagron	Palmitato de ascorbila	18A10-B03	1
Fagron	Palmitato de ascorbila	18A10B03344364	1
Fagron	Palmitato de ascorbila	18A10-B03-344364	23
Fagron	Palmitato de ascorbila	18A10-B03-525701	7
Fagron	Palmitato de ascorbila	18A10-B23-525701	1
Fagron	Palmitato de ascorbila	18B12-B09	3
Fagron	Palmitato de ascorbila	18B-12-B09-001	1
Fagron	Palmitato de ascorbila	18B12-B09-348867	14
Fagron	Palmitato de ascorbila	18B12-B09-3488670092	1
Fagron	Palmitato de ascorbila	18B12B09525719	1
Fagron	Palmitato de ascorbila	18B12-B09-525719	9
Fagron	Palmitato de ascorbila	18B12-B09-525720	5
Fagron	Palmitato de ascorbila	18B12-B09-525721	5
Fagron	Palmitato de ascorbila	18b12-B09-525799	1
Fagron	Palmitato de ascorbila	18B12-B09525799	1
Fagron	Palmitato de ascorbila	18B12-B09-525799	4
Fagron	Palmitato de ascorbila	18B12-B09-525820	2
Fagron	Palmitato de ascorbila	18B12-B09-525836	3
Fagron	Palmitato de ascorbila	18B12-B09-525888	2
Fagron	Palmitato de ascorbila	18B12-B09-525889	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Palmitato de ascorbila	18B12-B09-52889	1
Fagron	Palmitato de ascorbila	18B12-B09-528899	1
Fagron	Palmitato de ascorbila	18I22-B03-525911	1
Fagron	Palmitato de ascorbila	18I22-B03-525967	1
Fagron	Palmitato de ascorbila	18J22-B03	9
Fagron	Palmitato de ascorbila	18J22-B03_525967	1
Fagron	Palmitato de ascorbila	18j22-b03-355582	2
Fagron	Palmitato de ascorbila	18J22-B03-355582	6
Fagron	Palmitato de ascorbila	18J22-B03-357638	3
Fagron	Palmitato de ascorbila	18J22-B03-361032	1
Fagron	Palmitato de ascorbila	18J22-B03-525911	1
Fagron	Palmitato de ascorbila	18J22-B03525967	1
Fagron	Palmitato de ascorbila	18J22-B03-525967	5
Fagron	Palmitato de ascorbila	18J22-B03-526006	3
Fagron	Palmitato de ascorbila	18J22-B03-529967	1
Fagron	Palmitato de ascorbila	19/12-F02	1
Fagron	Palmitato de ascorbila	19112-F02-526151	1
Fagron	Palmitato de ascorbila	1912-F02	1
Fagron	Palmitato de ascorbila	19-12F02	1
Fagron	Palmitato de ascorbila	1912-F02364765	1
Fagron	Palmitato de ascorbila	1912-F02-521699	1
Fagron	Palmitato de ascorbila	19D25	1
Fagron	Palmitato de ascorbila	19D25-B04	18
Fagron	Palmitato de ascorbila	19d25b04361254	1
Fagron	Palmitato de ascorbila	19D25-B04-361254	24
Fagron	Palmitato de ascorbila	19D25-B04-361255	1
Fagron	Palmitato de ascorbila	19D25-B04-362604	7
Fagron	Palmitato de ascorbila	19D25-B04-526038	10
Fagron	Palmitato de ascorbila	19D25-B04-526062	8
Fagron	Palmitato de ascorbila	19D25-B04-526080	1
Fagron	Palmitato de ascorbila	19D25-B04-526092	6
Fagron	Palmitato de ascorbila	19D25-Bo4-361254	1
Fagron	Palmitato de ascorbila	19I12-F02	4
Fagron	Palmitato de ascorbila	19I12-F02-364756	1
Fagron	Palmitato de ascorbila	19I12-F02-364765	9
Fagron	Palmitato de ascorbila	19I12F02526151	1
Fagron	Palmitato de ascorbila	19I12-F02-526151	2
Fagron	Palmitato de ascorbila	19I12-F02-526152	4
Fagron	Palmitato de ascorbila	19I12F02526170	1
Fagron	Palmitato de ascorbila	19I12-F02-526199	1
Fagron	Palmitato de ascorbila	19K12-K03	1
Fagron	Palmitato de ascorbila	19l12-F02	1
Fagron	Palmitato de ascorbila	19O25-B04	1
Fagron	Palmitato de ascorbila	20/01-F04-373583	1
Fagron	Palmitato de ascorbila	2001-F04	2
Fagron	Palmitato de ascorbila	20101-F04-33584	1
Fagron	Palmitato de ascorbila	20101-F04-373584	1
Fagron	Palmitato de ascorbila	20101-F04-526393	1
Fagron	Palmitato de ascorbila	20A17F02	2
Fagron	Palmitato de ascorbila	20A17-F02	13
Fagron	Palmitato de ascorbila	20A17-F02-256273	1
Fagron	Palmitato de ascorbila	20A17F02368100	3
Fagron	Palmitato de ascorbila	20A17-F02-368100	20
Fagron	Palmitato de ascorbila	20A17-F02-526247	8
Fagron	Palmitato de ascorbila	20A17-F02-526273	12
Fagron	Palmitato de ascorbila	20A17-F02-526362	2
Fagron	Palmitato de ascorbila	20A17-FO2-526273	1
Fagron	Palmitato de ascorbila	20I01-04	1
Fagron	Palmitato de ascorbila	20I01-F04	7
Fagron	Palmitato de ascorbila	20I01-F04-373583	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Palmitato de ascorbila	20I01-F04-373584	4
Fagron	Palmitato de ascorbila	20I01-F04-526393	5
Fagron	Palmitato de ascorbila	20I0-F04-373584	1
Fagron	Palmitato de ascorbila	20l01-F04	1
Fagron	Palmitato de ascorbila	20l01-F04-373583	1
Fagron	Palmitato de ascorbila	20L07-F01	4
Fagron	Palmitato de ascorbila	20l07-f01-375723	1
Fagron	Palmitato de ascorbila	20L07-F01-375723	9
Fagron	Palmitato de ascorbila	20L07-F01-526454	1
Fagron	Palmitato de ascorbila	20L07-F01-526513	1
Fagron	Palmitato de ascorbila	20LO-F01-375723	1
Fagron	Palmitato de ascorbila	21E10-F02	11
Fagron	Palmitato de ascorbila	21E10-F02-378353	8
Fagron	Palmitato de ascorbila	21E10-F02-526522	5
Fagron	Palmitato de ascorbila	21E10-F02-526523	3
Fagron	Palmitato de ascorbila	21E10-F02-526524	1
Fagron	Palmitato de ascorbila	21E10-FO2-526625	1
Fagron	Palmitato de ascorbila	21E1O-259-0010	1
Fagron	Palmitato de ascorbila	21G17-804	1
Fagron	Palmitato de ascorbila	21G17-B04	5
Fagron	Palmitato de ascorbila	21G17-B04-213672	24
Fagron	Palmitato de ascorbila	21G17-BO4	1
Fagron	Palmitato de ascorbila	21G17-BO4-213672	1
Fagron	Palmitato de ascorbila	21L16B09217351	1
Fagron	Palmitato de ascorbila	21L16-B09-217351	5
Fagron	Palmitato de ascorbila	21L16-B09-221849	4
Fagron	Palmitato de ascorbila	21L16-B09W-217351	1
Fagron	Palmitato de ascorbila	21L16-Bo9-217351	1
Fagron	Palmitato de ascorbila	21L16-BO9-217351	1
Fagron	Palmitato de ascorbila	22F07-B01-22285	1
Fagron	Palmitato de ascorbila	22F07-B01-222885	3
Fagron	Palmitato de ascorbila	23061810	1
Fagron	Palmitato de ascorbila	24C13-B08-235298	1
Fagron	Palmitato de ascorbila	25/10/19Fr	1
Fagron	Palmitato de ascorbila	2OIO1-F04-373584	1
Fagron	Palmitato de ascorbila	2OIOF-F04-373583	1
Fagron	Palmitato de ascorbila	2OLO7-F01-375723	1
Fagron	Palmitato de ascorbila	525426	1
Fagron	Palmitato de ascorbila	525489	1
Fagron	Palmitato de ascorbila	525524	1
Fagron	Palmitato de ascorbila	525525	1
Fagron	Palmitato de ascorbila	925749	1
Fagron	Palmitato de ascorbila	A17-F02-368100	1
Fagron	Palmitato de ascorbila	BO4-2136702	1
Fagron	Palmitato de ascorbila	F01-3757203	3
Fagron	Palmitato de ascorbila	F02-3681000	1
Fagron	Palmitato de ascorbila	F02-3783503	3
Fagron	Palmitato de ascorbila	F02-5265203	1
Fagron	Palmitato de ascorbila	F04-3735803	2
Fagron	Palmitato de ascorbila	F04-3735804	2
Fagron	Palmitato de ascorbila	Fagron	1
Fagron	Palmitato de ascorbila	K45532790	2
Fagron	Palmitato de ascorbila	K47747490	1
Fagron	Palmitato de ascorbila	K48951290	1
Fagron	Palmitato de ascorbila	K48951390	2
Fagron	Palmitato de ascorbila	K49421190	6
Fagron	Palmitato de ascorbila	K50642890	4
Fagron	Palmitato de ascorbila	K50642890/19D25-B04	1
Fagron	Palmitato de ascorbila	k51125490	1
Fagron	Palmitato de ascorbila	K51125490	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Palmitato de ascorbila	UQ90606133	1
Fagron	Palmitato de ascorbila	UQ91006215	6
Fangro/4	Palmitato de ascorbila	19I12F02364765	1
Fargon/GEHE	Palmitato de ascorbila	19/12-F02-364765	1
Fargon/Noweda	Palmitato de ascorbila	18J22-B03-355582	1
Fargon/Sanacorp	Palmitato de ascorbila	19D25-B04-361254	1
Fargon	Palmitato de ascorbila	18A10-B03-344364	1
Fargon	Palmitato de ascorbila	19D25-B04-361254	1
Fargon	Palmitato de ascorbila	21E10-F02-526625	1
Fiebig	Palmitato de ascorbila	20I01-F04-373584	1
Gehe	Palmitato de ascorbila	18B12-B09-348867	1
Gehe	Palmitato de ascorbila	19I12-F02	1
GEHE	Palmitato de ascorbila	22F07-B01-222885	2
L12	Palmitato de ascorbila	18B12-B09	1
Merck	Palmitato de ascorbila	16130-B03	1
Merck	Palmitato de ascorbila	17E18-B06-334914	1
Merck	Palmitato de ascorbila	18J22-B03-357638	1
Merck	Palmitato de ascorbila	K50642890	1
Noweda / Fargon	Palmitato de ascorbila	20A17-F02-368100	1
Noweda 27.12.2019	Palmitato de ascorbila	19D25-B04-526062	1
Noweda	Palmitato de ascorbila	18J22-B03-525697	1
Noweda	Palmitato de ascorbila	18J22-B03-525943	1
Noweda	Palmitato de ascorbila	19D25-B04-362604	1
Noweda	Palmitato de ascorbila	20A17-F02-368100	1
Noweda	Palmitato de ascorbila	23A09-804-228316	1
Noweda	Palmitato de ascorbila	K50642890	1
Noweda_22.01.2020	Palmitato de ascorbila	19D25-B04-526038	1
PHOENIX 30.06.2014	Palmitato de ascorbila	UQ21206229	1
Phoenix	Palmitato de ascorbila	18812-B09-525720	2
Phoenix	Palmitato de ascorbila	18B12-B09	2
Phoenix	Palmitato de ascorbila	18J22-B03-357638	1
Phoenix	Palmitato de ascorbila	21L16-B09-221849	1
Phoenix	Palmitato de ascorbila	23A09-B04-228316	1
Phoenix	Palmitato de ascorbila	F04-3735803	1
Phönix/Bionorica	Palmitato de ascorbila	18A10-B03-344364	1
Phönix	Palmitato de ascorbila	17H04-B01-52632	1
PHÖNIX	Palmitato de ascorbila	18a10-B03-344364	1
Phönix	Palmitato de ascorbila	20l01-F04-373583	1
Phönix	Palmitato de ascorbila	21L16-B09-221849	1
Sanacorp	Palmitato de ascorbila	137-66-6	1
Sanacorp	Palmitato de ascorbila	17H04-B01	1
Sanacorp	Palmitato de ascorbila	18B12-B09	1
Sanacorp	Palmitato de ascorbila	19D25-B04-361254	2
Sanacorp	Palmitato de ascorbila	20I01-F04-526393	2
Sanacorp	Palmitato de ascorbila	21g17-b04-213672	1
Sanacorp	Palmitato de ascorbila	22F07-B01-222885	1

- 235 369 spectra from 1514 *Apo-Ident* customers from a total of 49 029 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Palmitato de ascorbila* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Palmitato de ascorbila* and it was

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	440	0	201 644
Type C	0	689	9	235 369

The substance/substance group *Palmitato de ascorbila* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	98.7106 % (> 98.2808 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21053	21053	0,00	87,04
21665	21053	38,94	85,47
21851	21053	43,39	86,72
23520	21053	26,65	87,83
24665	21053	18,58	87,70
25583	21053	36,73	87,70
27471	21053	44,47	87,61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pancreatina, pulverizada**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20976-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pancreatina, pulverizada; Pancreatis pulvis

Special notes

When selecting the *Pancreatina, pulverizada* substance/substance group, the following information is displayed to the user:

- Observação: Atualmente indisponível nos principais fabricantes farmacêuticos. Por isso, não é possível fazer a manutenção do lote no momento.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pancreatina, pulverizada	5	1	2

Second-stage model

For differentiation of the substance/substance group *Pancreatina, pulverizada* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pancreatina, pulverizada* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Lactose monoidratada	58,33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pancreatina, pulverizada* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pancreatina, pulverizada*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pancreatina, pulverizada	13118902	20976	40	1402190
Caelo	Pancreatina, pulverizada	13395203	21481	60	20131218
Caelo	Pancreatina, pulverizada	161397	22482	60	20160527*
Caelo	Pancreatina, pulverizada	16139708	23757	40	20160527
Caelo	Pancreatina, pulverizada	16139708	23758	40	20160527
Caelo	Pancreatina, pulverizada	20002501001	25520	40	20200929

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 280 spectra of 6 reference samples from the substance/substance group *Pancreatina, pulverizada*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 682 spectra from a total of 2837 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Pancreatina, pulverizada*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pancreatina, pulverizada	173226	23797	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Pancreatina, pulverizada*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Pancreatina, pulverizada	17322602	1
Caelo	Pancreatina, pulverizada	17322611	1

- 236 065 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pancreatina, pulverizada* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pancreatina, pulverizada* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	40	0	202 044
Type C	0	2	0	236 065

The substance/substance group *Pancreatina, pulverizada* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9013 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20976	20976	0,00	142,30
21481	22482	14,42	124,04
22482	22482	0,00	88,57
23757	22482	5,97	93,86
23758	22482	6,13	90,59
25520	22482	14,08	109,08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pantotenato de cálcio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20395-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pantotenato de cálcio; Calcii pantothenas

Special notes

When selecting the *Pantotenato de cálcio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pantotenato de cálcio	11	10	78

Second-stage model

For differentiation of the substance/substance group *Pantotenato de cálcio* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pantotenato de cálcio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	18,40	13,04
Sulfato de colistina	53,28	16,07
⋮	⋮	⋮
Bacitracina	59,49	15,49
Metilcobalamina	>50	34,15
Anfotericina B	>50	41,16
Cianocobalamina	>50	52,64
Nistatina	>50	56,76
Gelatina, branca	>50	58,17
Riboflavina	>50	61,84
Triancinolona	>50	67,61
Estradiol hemi-hidratado	>50	78,19
Vitamina E acetato pó 50%	>50	82,21
Levedura de selênio	>50	87,36
Glicerofosfato de cálcio	>50	95,43
Estriol	>50	108,61
Carmelose sódica	>50	128,33
Bromidrato de hioscina	>50	129,34
SyrSpend® SF Alka	>50	156,90
Tosilcloramida sódica	>50	163,34
Amido de arroz	>50	192,84
SyrSpend® SF pH4 neo	>50	227,36
Ácido oxálico	>50	249,76
Goma arábica, dispersão seca	>50	261,69
Amido de milho	>50	281,12
SyrSpend® SF pH4	>50	307,09
Fécula de batata	>50	383,72
Maltodextrina	>50	388,25
Amido de trigo	>50	389,13
Frutose	>50	407,10

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pantotenato de cálcio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pantotenato de cálcio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pantotenato de cálcio	14208012	21765	60	20140722
Caelo	Pantotenato de cálcio	173352	24045	40	20180202*
Euro OTC	Pantotenato de cálcio	1305034-01	21243	40	20130617
Euro OTC	Pantotenato de cálcio	1509024	21901	60	20151005*
Euro OTC	Pantotenato de cálcio	1603042	22551	40	20160429*
Euro OTC	Pantotenato de cálcio	1607023	22691	40	20160809*
Euro OTC	Pantotenato de cálcio	1702018	23153	40	20170330*
Euro OTC	Pantotenato de cálcio	1711003	23890	40	20171123*
Euro OTC	Pantotenato de cálcio	2008019	25296	40	20200921*
Euro OTC	Pantotenato de cálcio	2101037	25592	40	20210304*
Fagron	Pantotenato de cálcio	13H28-N11	21233	40	20130916

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Pantotenato de cálcio*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 152 482 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 450 spectra of 13 reference samples from the substance/substance group *Pantotenato de cálcio*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pantotenato de cálcio	162516	23363	40
Caelo	Pantotenato de cálcio	15344217	23717	40
Caelo	Pantotenato de cálcio	21003241008	26303	30
Caelo	Pantotenato de cálcio	23000511	26724	40
Euro OTC	Pantotenato de cálcio	1803014	24081	40
Euro OTC	Pantotenato de cálcio	1809014	24312	40
Euro OTC	Pantotenato de cálcio	1902032	24479	40
Euro OTC	Pantotenato de cálcio	2003007	25241	40
Euro OTC	Pantotenato de cálcio	2111014	25873	50
Euro OTC	Pantotenato de cálcio	2311018	27070	40
Caelo	Pantotenato de cálcio	21003241008	26303SI	20
Caelo	Pantotenato de cálcio	23000511	26724SI	20
Euro OTC	Pantotenato de cálcio	2111014	25873SI	10

- 201 634 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 198 spectra from 85 *Apo-Ident* customers from 82 batches from the substance/substance group *Pantotenato de cálcio*.

- Among them are spectra of independent samples from 78 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Pantotenato de cálcio	21003241015	1
	Pantotenato de cálcio	2111014-01	1
	Pantotenato de cálcio	22002458007	1
	Pantotenato de cálcio	23000511	1
	Pantotenato de cálcio	2301036-01	2
AHD	Pantotenato de cálcio	15344221	1
Anzag/Anzag 26.07.18	Pantotenato de cálcio	1803017-01	1
Caelo	Pantotenato de cálcio		1
Caelo	Pantotenato de cálcio	1013Q-03022	1
Caelo	Pantotenato de cálcio	11105731	1
Caelo	Pantotenato de cálcio	12236622	1
Caelo	Pantotenato de cálcio	12340808	3
Caelo	Pantotenato de cálcio	12340809	1
Caelo	Pantotenato de cálcio	12340819	2
Caelo	Pantotenato de cálcio	12340832	1
Caelo	Pantotenato de cálcio	12340846	1
Caelo	Pantotenato de cálcio	12340859	1
Caelo	Pantotenato de cálcio	1410011-01	1
Caelo	Pantotenato de cálcio	1410011-02	1
Caelo	Pantotenato de cálcio	14208004	1
Caelo	Pantotenato de cálcio	1509024-01	1
Caelo	Pantotenato de cálcio	15344207	1
Caelo	Pantotenato de cálcio	15344214	1
Caelo	Pantotenato de cálcio	1603042-01	1
Caelo	Pantotenato de cálcio	1607023-01	2
Caelo	Pantotenato de cálcio	16251608	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Pantotenato de cálcio	1711003-01	1
Caelo	Pantotenato de cálcio	17335208	5
Caelo	Pantotenato de cálcio	17335209	1
Caelo	Pantotenato de cálcio	18174608	1
Caelo	Pantotenato de cálcio	19057402	1
Caelo	Pantotenato de cálcio	19067402	2
Caelo	Pantotenato de cálcio	19067404	1
Caelo	Pantotenato de cálcio	19067405	2
Caelo	Pantotenato de cálcio	190751002	5
Caelo	Pantotenato de cálcio	190751004	3
Caelo	Pantotenato de cálcio	192718003	3
Caelo	Pantotenato de cálcio	192718004	5
Caelo	Pantotenato de cálcio	20004234001	3
Caelo	Pantotenato de cálcio	20004234003	1
Caelo	Pantotenato de cálcio	20004252009	1
Caelo	Pantotenato de cálcio	21003241008	2
Caelo	Pantotenato de cálcio	27111303	1
Caelo	Pantotenato de cálcio	8041407	1
Caesar & Loretz GmbH...	Pantotenato de cálcio	20004252012	1
Caesar & Loretz GmbH...	Pantotenato de cálcio	21003241008	3
Caesar & Loretz GmbH...	Pantotenato de cálcio	19067404	1
Caesar & Loretz GmbH/Phoe	Pantotenato de cálcio	20004234001	2
Caesar & Loretz GmbH...	Pantotenato de cálcio	190751002	1
Caesar & Loretz GmbH...	Pantotenato de cálcio	192718004	1
Caesar & Loretz GmbH	Pantotenato de cálcio	17335209	2
Caesar & Loretz GmbH	Pantotenato de cálcio	19067404	1
Caesar & Loretz GmbH	Pantotenato de cálcio	190751002	5
Caesar & Loretz GmbH	Pantotenato de cálcio	192718003	1
Caesar & Loretz GmbH	Pantotenato de cálcio	192718004	2
Caesar & Loretz GmbH	Pantotenato de cálcio	20004252009	2
Caesar/Gehe	Pantotenato de cálcio	17335209	2
EuRho/sanacorp	Pantotenato de cálcio	1803014-01	1
Euro OTC	Pantotenato de cálcio	10021505	1
Euro OTC	Pantotenato de cálcio	1111025-01	1
Euro OTC	Pantotenato de cálcio	1209022-01	1
Euro OTC	Pantotenato de cálcio	1209022-02	1
Euro OTC	Pantotenato de cálcio	1209022-02pzn	1
Euro OTC	Pantotenato de cálcio	130503401	2
Euro OTC	Pantotenato de cálcio	1305034-01	4
Euro OTC	Pantotenato de cálcio	1312027-01	3
Euro OTC	Pantotenato de cálcio	1410011-01	1
Euro OTC	Pantotenato de cálcio	1410011-02	3
Euro OTC	Pantotenato de cálcio	1509024-01	3
Euro OTC	Pantotenato de cálcio	1603042-01	4
Euro OTC	Pantotenato de cálcio	1607023-01	3
Euro OTC	Pantotenato de cálcio	1702018-01	3
Euro OTC	Pantotenato de cálcio	17021401	1
Euro OTC	Pantotenato de cálcio	1711003-01	7
Euro OTC	Pantotenato de cálcio	1803014-01	4
Euro OTC	Pantotenato de cálcio	1809014-01	2
Euro OTC	Pantotenato de cálcio	18111707	1
Euro OTC	Pantotenato de cálcio	1902023-01	1
Euro OTC	Pantotenato de cálcio	190203201	1
Euro OTC	Pantotenato de cálcio	1902032-01	2
Euro OTC	Pantotenato de cálcio	190203202	1
Euro OTC	Pantotenato de cálcio	1902032-02	4
Euro OTC	Pantotenato de cálcio	2001037-01	1
Euro OTC	Pantotenato de cálcio	200300701	1
Euro OTC	Pantotenato de cálcio	2003007-01	6
Euro OTC	Pantotenato de cálcio	2008019-01	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Pantotenato de cálcio	201037-01	1
Euro OTC	Pantotenato de cálcio	2101037-01	6
Euro OTC	Pantotenato de cálcio	2111014-01	7
Euro OTC	Pantotenato de cálcio	2111014-02	1
Euro OTC	Pantotenato de cálcio	2301036-01	1
Euro OTC	Pantotenato de cálcio	5121405	1
Euro OTC	Pantotenato de cálcio	99142536W0	1
Euroo/Anzag	Pantotenato de cálcio	1509024-01	2
Fagron	Pantotenato de cálcio	1111025-01	1
Fagron	Pantotenato de cálcio	1111110405	1
Fagron	Pantotenato de cálcio	12F19-N07	1
Fagron	Pantotenato de cálcio	13H28-N11	1
Fagron	Pantotenato de cálcio	14G02-B10-297373	1
Gehe Pharma Handel	Pantotenato de cálcio	22002458006	1
Gehe	Pantotenato de cálcio	1004024-01	1
Hangzhou xinfu	Pantotenato de cálcio	2008019-01	2
Nachprüfung	Pantotenato de cálcio	123456	1
Noweda	Pantotenato de cálcio	14208012	1
Noweda	Pantotenato de cálcio	TL017107823	1
Sanacorp	Pantotenato de cálcio	17335203	1

- 235 869 spectra from 1515 *Apo-Ident* customers from a total of 49 179 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pantotenato de cálcio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pantotenato de cálcio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	450	0	201 634
Type C	0	198	0	235 869

The substance/substance group *Pantotenato de cálcio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.9697 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21233	23890	20,37	60,33
21243	24045	15,83	58,25
21765	24045	11,55	58,25
21901	21901	0,00	59,49
22551	22551	0,00	36,93
22691	22691	0,00	41,68
23153	23153	0,00	59,36
23890	23890	0,00	59,68
24045	24045	0,00	58,45
25296	25296	0,00	63,36
25592	25592	0,00	49,51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Paracetamol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20972-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Paracetamol; Paracetamolum

Special notes

When selecting the *Paracetamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Paracetamol	10	9	81

Second-stage model

For differentiation of the substance/substance group *Paracetamol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Paracetamol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	118,24	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Paracetamol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Paracetamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Paracetamol	15075706	22608	40	20150424
Caelo	Paracetamol	15075707	22822	40	20150424
Caelo	Paracetamol	191851	24889	40	20190827*
Caelo	Paracetamol	20001174	25629	40	20200624*
Caelo	Paracetamol	22002446	26370	40	20220818*
Caelo	Paracetamol	22002446	26370SI	20	20220818*
Euro OTC	Paracetamol	1111024-02	21598	60	20120123
Fagron	Paracetamol	13D30-N03	20972	40	1402271
Fagron	Paracetamol	13D16-N08	20973	40	1402296
Fagron	Paracetamol	13G23-N03	20974	40	1402297
Fagron	Paracetamol	21K05-B01-223625	26379	40	20220307
Fagron	Paracetamol	21K05-B01-223625	26379SI	20	20220307

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 12 reference samples from the substance/substance group *Paracetamol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 502 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 11 reference samples from the substance/substance group *Paracetamol*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Paracetamol	170284	23852	40
Caelo	Paracetamol	180830	24053	40
Caelo	Paracetamol	22003365	26492	40
Caelo	Paracetamol	22003972	26497	40
Euro OTC	Paracetamol	2003059	25144	40
Euro OTC	Paracetamol	2211002	26426	40
Euro OTC	Paracetamol	2301037	26588	40
Euro OTC	Paracetamol	2301022	26597	40
Euro OTC	Paracetamol	2401012	27142	40
Caelo	Paracetamol	22003365	26492SI	20
Caelo	Paracetamol	22003972	26497SI	20

- 201 684 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 212 spectra from 120 *Apo-Ident* customers from 83 batches from the substance/substance group *Paracetamol*.

- Among them are spectra of independent samples from 80 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Paracetamol	22002805001	1
	Paracetamol	22003365004	1
	Paracetamol	230102201	1
	Paracetamol	2301022-01	3
	Paracetamol	231022-01	1
Anzag	Paracetamol	22003972003	1
Caeleo/ Kehr	Paracetamol	19185102	4
Caeleo/ Kehr	Paracetamol	20003925002	3
Caelo	Paracetamol		1
Caelo	Paracetamol	10065102	1
Caelo	Paracetamol	10325020	1
Caelo	Paracetamol	11300108	1
Caelo	Paracetamol	11300120	2
Caelo	Paracetamol	13082005	1
Caelo	Paracetamol	13082010	3
Caelo	Paracetamol	13082011	1
Caelo	Paracetamol	15075704	4
Caelo	Paracetamol	15075708	1
Caelo	Paracetamol	15217701	1
Caelo	Paracetamol	15217704	1
Caelo	Paracetamol	15217706	1
Caelo	Paracetamol	15217708	1
Caelo	Paracetamol	15217710	5
Caelo	Paracetamol	15217712	2
Caelo	Paracetamol	15245901	3
Caelo	Paracetamol	15245902	1
Caelo	Paracetamol	17028409	4
Caelo	Paracetamol	17028411	3
Caelo	Paracetamol	18018602	1
Caelo	Paracetamol	18018604	1
Caelo	Paracetamol	18083003	4
Caelo	Paracetamol	18083005	5
Caelo	Paracetamol	18083006	4
Caelo	Paracetamol	18083007	1
Caelo	Paracetamol	18083012	2
Caelo	Paracetamol	18083014	5
Caelo	Paracetamol	1814U-02045	1
Caelo	Paracetamol	1912M-02045	1
Caelo	Paracetamol	191851001	1
Caelo	Paracetamol	191851002	2
Caelo	Paracetamol	191851004	6
Caelo	Paracetamol	20001174002	3
Caelo	Paracetamol	20003925001	1
Caelo	Paracetamol	20003925002	2
Caelo	Paracetamol	20003925004	5
Caelo	Paracetamol	20003925005	2
Caelo	Paracetamol	20003925007	2
Caelo	Paracetamol	20003925008	1
Caelo	Paracetamol	20003925009	1
Caelo	Paracetamol	20003925011	1
Caelo	Paracetamol	20003925014	1
Caelo	Paracetamol	20003925015	2
Caelo	Paracetamol	20003925016	2
Caelo	Paracetamol	20003925018	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Paracetamol	2000392504	1
Caelo	Paracetamol	2000395016	1
Caelo	Paracetamol	211222	1
Caelo	Paracetamol	22002446004	2
Caelo	Paracetamol	22002446005	3
Caelo	Paracetamol	22002805001	8
Caelo	Paracetamol	22002805005	1
Caelo	Paracetamol	22003365002	2
Caelo	Paracetamol	2815I-02045	1
Caelo	Paracetamol	5116I-02045	1
Caesar & Loretz GmbH...	Paracetamol	22002805002	2
Caesar & Loretz GmbH...	Paracetamol	22002805001	1
Caesar & Loretz GmbH...	Paracetamol	18083012	1
Caesar & Loretz GmbH/AHD	Paracetamol	22002446002	1
Caesar & Loretz GmbH/Gehe	Paracetamol	20003925009	1
Caesar & Loretz GmbH/Kehr	Paracetamol	22002805001	1
Caesar & Loretz GmbH...	Paracetamol	22002805007	1
Caesar & Loretz GmbH...	Paracetamol	20003925005	2
Caesar & Loretz GmbH...	Paracetamol	22002805002	1
Caesar & Loretz GmbH	Paracetamol	18083003	1
Caesar & Loretz GmbH	Paracetamol	18083006	1
Caesar & Loretz GmbH	Paracetamol	18083008	1
Caesar & Loretz GmbH	Paracetamol	191851002	2
Caesar & Loretz GmbH	Paracetamol	191851004	1
Caesar & Loretz GmbH	Paracetamol	20003925017	1
Caesar & Loretz GmbH	Paracetamol	22002446002	1
Caesar & Loretz GmbH	Paracetamol	22002446004	3
Caesar & Loretz GmbH	Paracetamol	22002446005	2
Caesar & Loretz GmbH	Paracetamol	22002805001	1
Caesar & Loretz GmbH	Paracetamol	22002805002	1
Caesar & Loretz GmbH	Paracetamol	22003365002	1
Caesar & Loretz GmbH	Paracetamol	22003365004	1
Caesar & Loretz GmbH	Paracetamol	22003365007	1
Caesar & Loretz Hilden	Paracetamol	18083006	1
Euro OTC	Paracetamol	1111024-01	1
Euro OTC	Paracetamol	1111024-02	1
Euro OTC	Paracetamol	17028409	1
Euro OTC	Paracetamol	2003059-01	3
Euro OTC	Paracetamol	2003059-02	1
Euro OTC	Paracetamol	2003059-03	3
Euro OTC	Paracetamol	200305904	2
Euro OTC	Paracetamol	2211002-01	5
Euro OTC	Paracetamol	2301022-01	1
Euro OTC	Paracetamol	3003059-02	1
Fagron	Paracetamol		1
Fagron	Paracetamol	13L16-B02-322725	1
Fagron	Paracetamol	17H17-B03	2
Fagron	Paracetamol	17H17-B03-359484	1
Fagron	Paracetamol	17H17-B03-367674	1
Fagron	Paracetamol	20F18-F02-224205	4
Fagron	Paracetamol	20F18-F02-374185	1
Gehe	Paracetamol	20003925007	1
Gehe	Paracetamol	2301022-01	1
Jenne	Paracetamol	15245901	1
Kehr	Paracetamol	20003925005	1
Nachprüfung	Paracetamol	15245901	2
Noweda	Paracetamol	18018602	2
Noweda	Paracetamol	2003059-02	1
Noweda	Paracetamol	20F18-F02-224205	1
Noweda	Paracetamol	2211002-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Paracetamol	22002805001	1
Sanacorp	Paracetamol	22002805001	1

- 235 855 spectra from 1515 *Apo-Ident* customers from a total of 49 175 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Paracetamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Paracetamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	400	0	201 684
Type C	0	207	5	235 855

The substance/substance group *Paracetamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.9007 %)	97.6415 % (> 96.2264 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20972	20972	0,00	202,49
20973	20973	0,00	201,65
20974	20974	0,00	215,45
21598	24889	8,92	201,27

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22608	24889	7,60	199,11
22822	25629	8,23	202,96
24889	24889	0,00	207,78
25629	25629	0,00	205,86
26370	26370	0,00	203,62
26379	20974	26,25	215,84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pectina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005975-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pectina

Special notes

When selecting the *Pectina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pectina	2	1	0

Second-stage model

For differentiation of the substance/substance group *Pectina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pectina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dibásico de sódio di-hidratado	60,71	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pectina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pectina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pectina	21003677	26013	40	20220107*
Caelo	Pectina	24001504	27318	40	20240717*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Pectina*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 4 reference samples from the substance/substance group *Pectina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pectina	23000147	27108	40
Caelo	Pectina	21003677	26013SI†	10
Caelo	Pectina	23000147	27108SI	20
Caelo	Pectina	24001504	27318SI†	20

- 201 994 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Pectina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pectina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pectina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	90	0	201 994
Type C	0	0	0	236 067

The substance/substance group *Pectina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26013	26013	0,00	96,35
27318	27318	0,00	89,43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Piridoxal-5-fosfato**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20830-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Piridoxal-5-fosfato

Special notes

When selecting the *Piridoxal-5-fosfato* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Piridoxal-5-fosfato	9	5	11

Second-stage model

For differentiation of the substance/substance group *Piridoxal-5-fosfato* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Piridoxal-5-fosfato* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	47,69	–
Proteinato de prata	57,86	–
⋮	⋮	⋮
Citrato de sódio	>50	74,58
Levocarnitina	>50	177,40
Capsaicina	>50	190,00
Alfaestradiol	>50	204,76
Cloridrato de oxibutinina	>50	208,83
Prednicarbato	>50	322,01
Cloridrato de quinina di-hidratado	>50	372,95
Cloridrato de ciprofloxacina	>50	488,59
Tetracaína	>50	488,89
Metoxisaleno	>50	493,54
Heparina sódica	>50	523,26
Acetato de ciproterona	>50	549,09
Acetato de noretisterona	>50	616,47
Cloridrato de amitriptilina	>50	857,06
Valina	>50	1083,81
Triclosan	>50	1127,95
Amifampridina	>50	1335,95
Sacarose	>50	1556,34

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Piridoxal-5-fosfato* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Piridoxal-5-fosfato*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Piridoxal-5-fosfato	1302029-01	20830	40	8897
Euro OTC	Piridoxal-5-fosfato	1302029-01	21097	40	20130315
Euro OTC	Piridoxal-5-fosfato	1701015	23133	40	20170220*
Euro OTC	Piridoxal-5-fosfato	1701015-01	23276	40	20170220
Euro OTC	Piridoxal-5-fosfato	1808030	24329	40	20181019*
Euro OTC	Piridoxal-5-fosfato	1902022	24542	40	20190320*
Euro OTC	Piridoxal-5-fosfato	1908001	24833	40	20190903*
Euro OTC	Piridoxal-5-fosfato	1910027	24923	40	20191217*
Euro OTC	Piridoxal-5-fosfato	2102013	25594	40	20210317*
Euro OTC	Piridoxal-5-fosfato	2104017	25674	40	20210602*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Piridoxal-5-fosfato*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Piridoxal-5-fosfato*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Piridoxal-5-fosfato	1711030	23877	40
Euro OTC	Piridoxal-5-fosfato	2001043	25130	40
Euro OTC	Piridoxal-5-fosfato	2003038	25151	40
Euro OTC	Piridoxal-5-fosfato	2110012	25876	50
Euro OTC	Piridoxal-5-fosfato	2211016	26589	40
Euro OTC	Piridoxal-5-fosfato	2110012	25876SI	10
Euro OTC	Piridoxal-5-fosfato	2211016	26589SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 844 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 12 *Apo-Ident* customers from 13 batches from the substance/substance group *Piridoxal-5-fosfato*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Denk	Piridoxal-5-fosfato	20171202	1
Denk	Piridoxal-5-fosfato	C041402802	1
EuRho	Piridoxal-5-fosfato	2003038-01	4
Euro OTC	Piridoxal-5-fosfato	1701015-01	3
Euro OTC	Piridoxal-5-fosfato	1711030-01	2
Euro OTC	Piridoxal-5-fosfato	1808030	1
Euro OTC	Piridoxal-5-fosfato	1808030-01	2
Euro OTC	Piridoxal-5-fosfato	1808030-02	4
Euro OTC	Piridoxal-5-fosfato	1902022-01	1
Euro OTC	Piridoxal-5-fosfato	1908001-01	4
Euro OTC	Piridoxal-5-fosfato	2003038-01	1
Euro OTC	Piridoxal-5-fosfato	2003038-02	1
Fagron	Piridoxal-5-fosfato	2001043-01	1
Inresa Arznei	Piridoxal-5-fosfato	13100411	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Piridoxal-5-fosfato* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Piridoxal-5-fosfato* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	240	0	201 844
Type C	0	27	0	236 040

The substance/substance group *Piridoxal-5-fosfato* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20830	20830	0,00	90,72
21097	20830	6,90	84,70
23133	23133	0,00	80,90
23276	20830	14,84	97,14
24329	24329	0,00	164,55
24542	24542	0,00	128,35
24833	24833	0,00	132,18
24923	24923	0,00	146,88
25594	25594	0,00	131,46
25674	25674	0,00	123,68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Poloxâmero**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20540-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Poloxâmero; Poloxamera

Special notes

When selecting the *Poloxâmero* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Poloxâmero	6	6	46

Second-stage model

For differentiation of the substance/substance group *Poloxâmero* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Poloxâmero* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Monoestearato de glicerol, emulsionante	96,55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Poloxâmero* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Poloxâmero*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Poloxâmero	14196101	21652	60	AR-14-FG-013090-01
Caelo	Poloxâmero	16242605	23257	40	20160915
Caelo	Poloxâmero	20003669003	25509	40	20201117
Caelo	Poloxâmero	22003362006	26746	40	20230208
Caelo	Poloxâmero	22003362006	26746SI	20	20230208
Caelo	Poloxâmero	23001663	27115	40	20231207*
Caelo	Poloxâmero	23001663	27115SI	20	20231207*
Fagron	Poloxâmero	14G17-B03-296866	21726	60	20140806

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Poloxâmero*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Poloxâmero*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Poloxâmero	170486	23311	40
Caelo	Poloxâmero	172921	23810	40
Caelo	Poloxâmero	181607	24219	40
Caelo	Poloxâmero	182636	24358	40
Caelo	Poloxâmero	21001523004	25980	40
Caelo	Poloxâmero	24002242	27437	40
Caelo	Poloxâmero	21001523004	25980SI	10

- 201 834 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 136 spectra from 89 *Apo-Ident* customers from 50 batches from the substance/substance group *Poloxâmero*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Poloxâmero	22003362006	1
	Poloxâmero	22003362007	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Poloxâmero	22003362010	1
Anzag	Poloxâmero	22003362006	1
Caelo	Poloxâmero	12286801	2
Caelo	Poloxâmero	12286805	1
Caelo	Poloxâmero	12286806	1
Caelo	Poloxâmero	13133201	1
Caelo	Poloxâmero	13133203	2
Caelo	Poloxâmero	13133207	1
Caelo	Poloxâmero	14196101	2
Caelo	Poloxâmero	14196104	1
Caelo	Poloxâmero	14196105	1
Caelo	Poloxâmero	14196108	2
Caelo	Poloxâmero	14359501	1
Caelo	Poloxâmero	15183102	2
Caelo	Poloxâmero	15397802	5
Caelo	Poloxâmero	16189301	1
Caelo	Poloxâmero	16189302	4
Caelo	Poloxâmero	16242601	3
Caelo	Poloxâmero	16242605	3
Caelo	Poloxâmero	162426056	1
Caelo	Poloxâmero	17048601	4
Caelo	Poloxâmero	17048606	2
Caelo	Poloxâmero	17292101	2
Caelo	Poloxâmero	18025101	13
Caelo	Poloxâmero	18160702	10
Caelo	Poloxâmero	18160704	4
Caelo	Poloxâmero	182636001	3
Caelo	Poloxâmero	18263601	4
Caelo	Poloxâmero	18263605	3
Caelo	Poloxâmero	18263607	4
Caelo	Poloxâmero	20000294001	3
Caelo	Poloxâmero	20003669003	8
Caelo	Poloxâmero	21001523001	4
Caelo	Poloxâmero	22003362002	1
Caesar & Loretz GmbH…	Poloxâmero	18263601	1
Caesar & Loretz GmbH/Gehe	Poloxâmero	18263607	1
Caesar & Loretz GmbH…	Poloxâmero	182636	1
Caesar & Loretz GmbH	Poloxâmero	15183102	1
Caesar & Loretz GmbH	Poloxâmero	182636002	3
Caesar & Loretz GmbH	Poloxâmero	18263601	1
Caesar & Loretz GmbH	Poloxâmero	18263607	1
Caesar & Loretz GmbH	Poloxâmero	20000294001	1
Caesar & Loretz GmbH	Poloxâmero	20003669003	2
Caesar & Loretz GmbH	Poloxâmero	21001523001	1
Caesar & Loretz GmbH	Poloxâmero	21001523004	2
Euro OTC	Poloxâmero	15397802	1
Fagron	Poloxâmero	12K23-N03	1
Fagron	Poloxâmero	13G29-N01	1
Fagron	Poloxâmero	13G29-NO1	1
Fagron	Poloxâmero	15A26-B03-303503	1
Fagron	Poloxâmero	315E-07027	1
Fagron	Poloxâmero	318A-07027	1
Fagron	Poloxâmero	5211Q-07027	1
Fagron	Poloxâmero	5315I-07027	1
Fagron	Poloxâmero	914I-07027	1
Fagron	Poloxâmero	WPWI610C	1
Noweda	Poloxâmero	18263607	1
Phonix	Poloxâmero	12/13-N10	1
Sanacorp	Poloxâmero	14196101	2
Sigma-Aldrich	Poloxâmero	BCBW9875	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 931 spectra from 1515 *Apo-Ident* customers from a total of 49 208 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Poloxâmero* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Poloxâmero* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	250	0	201 834
Type C	0	135	1	235 931

The substance/substance group *Poloxâmero* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	99.2647 % (> 97.0588 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21652	21652	0,00	128,26
21726	21652	6,54	128,12
23257	21652	8,83	129,34
25509	27115	11,88	130,40
26746	21652	16,89	130,73
27115	27115	0,00	130,17

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Povidona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20684-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Povidona; Povidonum

Special notes

When selecting the *Povidona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Povidona	15	8	57

Second-stage model

For differentiation of the substance/substance group *Povidona* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Povidona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Iodopovidona	27,69	11,08
Progesterona	69,45	54,06
⋮	⋮	⋮
Espironolactona	>50	46,09
Ácido fusídico	85,20	50,44
Propionato de testosterona	>50	73,01
Ubidecarenona	>50	126,19

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Povidona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Povidona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Povidona	12032714	20684	40	1402437
Caelo	Povidona	14142103	21378	40	AR-15-FG-000596-01
Caelo	Povidona	16307808	23255	40	AR-17-FG-015299-02
Caelo	Povidona	180276	24044	40	20180202*
Caelo	Povidona	191752	24746	40	20190717*
Caelo	Povidona	191276	24754	40	20190517*
Caelo	Povidona	20000212	25194	40	20200313*
Caelo	Povidona	20003415	25624	40	20201116*
Caelo	Povidona	21003749	26003	40	20220203*
Caelo	Povidona	23001270	26831	40	20230627*
Caelo	Povidona	24000976	27335	40	20240826*
Fagron	Povidona	12E22-N05	20770	40	1411537
Fagron	Povidona	13J21-N02	22731	40	AR-16-FG-019116-01
Fagron	Povidona	15C12-B02-323006	23265	40	1710348
Fagron	Povidona	21I30-B03-219629	26287	40	20220510

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 600 spectra of 15 reference samples from the substance/substance group *Povidona*. These samples are listed above in the *calibration samples* section. The reference samples come from 15 different batches.

- 152 362 spectra from a total of 2827 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 11 reference samples from the substance/substance group *Povidona*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Povidona	172091	23619	40
Caelo	Povidona	180766	24245	40
Caelo	Povidona	181820	24246	40
Caelo	Povidona	182383	24291	40
Caelo	Povidona	183000	24396	40
Caelo	Povidona	192500	24899	40
Caelo	Povidona	23002064	26953	40
Fagron	Povidona	23E05-B03-228683	26917	40
Caelo	Povidona	21003749	26003SI†	20
Caelo	Povidona	23001270	26831SI†	20
Fagron	Povidona	21I30-B03-219629	26287SI†	20

- 201 704 spectra from a total of 4034 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 184 spectra from 72 *Apo-Ident* customers from 60 batches from the substance/substance group *Povidona*.
- Among them are spectra of independent samples from 57 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Povidona	23001270003	1
21001192005	Povidona	21001192005	1
Alliance	Povidona	16307808	1
Alliance	Povidona	17209106	1
Alliance	Povidona	18112201	1
Audor Pharma	Povidona	18112201	1
Caelo	Povidona	12032714	1
Caelo	Povidona	12376301	1
Caelo	Povidona	13323407	2
Caelo	Povidona	14142103	1
Caelo	Povidona	14142109	3
Caelo	Povidona	14207508	3
Caelo	Povidona	14207511	4
Caelo	Povidona	14207515	1
Caelo	Povidona	14207517	1
Caelo	Povidona	15013721	1
Caelo	Povidona	15383101	3
Caelo	Povidona	15383102	1
Caelo	Povidona	15383103	2
Caelo	Povidona	16051101	2
Caelo	Povidona	16051102	1
Caelo	Povidona	16051103	1
Caelo	Povidona	16051104	1
Caelo	Povidona	16051108	2
Caelo	Povidona	16051110	1
Caelo	Povidona	16307802	1
Caelo	Povidona	16307808	1
Caelo	Povidona	163078085328	1
Caelo	Povidona	16307809	5
Caelo	Povidona	16307811	3
Caelo	Povidona	16307812	1
Caelo	Povidona	17209103	2
Caelo	Povidona	17209104	3
Caelo	Povidona	17209110	1
Caelo	Povidona	18024602	1
Caelo	Povidona	18027602	5
Caelo	Povidona	18112201	4
Caelo	Povidona	18182002	2
Caelo	Povidona	18238302	1
Caelo	Povidona	18300002	3
Caelo	Povidona	18300003	1
Caelo	Povidona	18300006	1
Caelo	Povidona	19127604	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Povidona	19175202	5
Caelo	Povidona	19175204	2
Caelo	Povidona	192500001	1
Caelo	Povidona	19500001	1
Caelo	Povidona	20000212001	10
Caelo	Povidona	20000212005	3
Caelo	Povidona	20001927003	1
Caelo	Povidona	20003415001	2
Caelo	Povidona	20003415004	1
Caelo	Povidona	20003415005	2
Caelo	Povidona	20003606003	1
Caelo	Povidona	21001192003	4
Caelo	Povidona	21001192005	1
Caelo	Povidona	21003749002	4
Caelo	Povidona	22001357001	4
Caesar & Loretz GmbH…	Povidona	20000212005	1
Caesar & Loretz GmbH…	Povidona	20003415005	1
Caesar & Loretz GmbH…	Povidona	20001927003	2
Caesar & Loretz GmbH…	Povidona	20003415001	1
Caesar & Loretz GmbH…	Povidona	20000212001	1
Caesar & Loretz GmbH…	Povidona	20003415001	4
Caesar & Loretz GmbH…	Povidona	20003415004	1
Caesar & Loretz GmbH…	Povidona	21001192003	1
Caesar & Loretz GmbH…	Povidona	21003749002	1
Caesar & Loretz GmbH/Sa	Povidona	20000212005	1
Caesar & Loretz GmbH…	Povidona	22001357001	4
Caesar & Loretz GmbH	Povidona	18112201	1
Caesar & Loretz GmbH	Povidona	18238302	1
Caesar & Loretz GmbH	Povidona	18300002	2
Caesar & Loretz GmbH	Povidona	18300006	1
Caesar & Loretz GmbH	Povidona	19127604	1
Caesar & Loretz GmbH	Povidona	19175202	1
Caesar & Loretz GmbH	Povidona	20000212001	1
Caesar & Loretz GmbH	Povidona	20000212005	2
Caesar & Loretz GmbH	Povidona	20001927003	4
Caesar & Loretz GmbH	Povidona	20003415001	3
Caesar & Loretz GmbH	Povidona	20003415004	3
Caesar & Loretz GmbH	Povidona	20003415005	3
Caesar & Loretz GmbH	Povidona	20003606001	1
Caesar & Loretz GmbH	Povidona	21001192003	1
Caesar & Loretz GmbH	Povidona	21001192005	5
Caesar & Loretz GmbH	Povidona	21003749002	5
Caesar & Loretz GmbH	Povidona	22001357001	3
Caesar & Loretz Hild…	Povidona	18300002	1
Caesar / Ebert	Povidona	15383101	2
Cealo	Povidona	4369127	1
Fagron	Povidona	11276509T0	1
Fagron	Povidona	15C12-B02-327866	1
Fagron	Povidona	24701988Q0	1
GEHE	Povidona	18112201	1
Gehe	Povidona	18300002	1
Phönix	Povidona	192500001	1
Sanacorp	Povidona	32470709T0	1

- 235 883 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Povidona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Povidona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	600	0	152 362
Type B	0	380	0	201 704
Type C	0	164	20	235 883

The substance/substance group *Povidona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	89.1304 % (> 87.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20684	20684	0,00	30,73
20770	20770	0,00	52,35
21378	21378	0,00	29,27
22731	22731	0,00	89,50
23255	23255	0,00	31,30
23265	23265	0,00	72,30
24044	24044	0,00	35,81
24746	24746	0,00	114,25
24754	24754	0,00	140,77
25194	25194	0,00	144,21
25624	25624	0,00	83,54
26003	26003	0,00	81,64
26287	26831	17,97	51,11
26831	26831	0,00	53,74
27335	27335	0,00	94,94

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prasterona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20703-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prasterona; Dehidroepiandrosterona; DHEA; Prasteronum

Special notes

When selecting the *Prasterona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prasterona	21	18	125

Second-stage model

For differentiation of the substance/substance group *Prasterona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prasterona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Valerato de estradiol	86,83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prasterona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prasterona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Prasterona	APZDHA16003-M	23931	40	1805404
Audor Pharma	Prasterona	APZDHAC17003MD	24412	40	20180119
Audor Pharma	Prasterona	APZDHAC18004D	24430	40	1906523
Euro OTC	Prasterona	1102036-01	20703	40	1404310
Euro OTC	Prasterona	1506011	21824	60	20150629*
Euro OTC	Prasterona	1602018	22506	30	20160301*
Euro OTC	Prasterona	1704012	23389	40	20170529*
Euro OTC	Prasterona	1707014	23695	40	20170829*
Euro OTC	Prasterona	1710035	23868	40	20171212*
Euro OTC	Prasterona	1712014	23893	40	20180115*
Euro OTC	Prasterona	1809009	24323	40	20181010*
Euro OTC	Prasterona	1907045	24853	40	20190905*
Euro OTC	Prasterona	1809009	24966	40	20191111*
Euro OTC	Prasterona	1910025	24967	40	20191111*
Euro OTC	Prasterona	2001038	25091	40	20200302*
Euro OTC	Prasterona	2102004	25537	40	20210224*
Euro OTC	Prasterona	2101011	25568	40	20210224*
Euro OTC	Prasterona	2301032	26513	39	20230202*
Fagron	Prasterona	13J10-B02-287175	20960	40	1404309
Fagron	Prasterona	15G14-B07-310827	21917	60	20150814
Fagron	Prasterona	16L13-B01-330724	23865	40	20161228
Fagron	Prasterona	22E25-F01-382686	26408	40	20220720

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 909 spectra of 22 reference samples from the substance/substance group *Prasterona*. These samples are listed above in the *calibration samples* section. The reference samples come from 21 different batches.
- 152 053 spectra from a total of 2821 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 800 spectra of 23 reference samples from the substance/substance group *Prasterona*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Prasterona	APZDHA16003-1MD	23932	40
Euro OTC	Prasterona	1702025	23147	40
Euro OTC	Prasterona	1805018	24137	40
Euro OTC	Prasterona	1809010	24318	40
Euro OTC	Prasterona	1901030	24453	40
Euro OTC	Prasterona	1901031	24454	40
Euro OTC	Prasterona	2005008	25152	40
Euro OTC	Prasterona	2005007	25153	40
Euro OTC	Prasterona	2201038	25955	40
Euro OTC	Prasterona	2203004	26100	30
Euro OTC	Prasterona	2206014	26216	40
Euro OTC	Prasterona	2209007	26344	40
Euro OTC	Prasterona	2301031	26594	40
Euro OTC	Prasterona	2311028	27003	40
Euro OTC	Prasterona	2408001	27393	40
Euro OTC	Prasterona	2408002	27394	40
Fagron	Prasterona	18C12-B01-347633	23990	40
Fagron	Prasterona	23K03-B04-231722	27033	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prasterona	2201038	25955SI	10
Euro OTC	Prasterona	2203004	26100SI	20
Euro OTC	Prasterona	2206014	26216SI	20
Euro OTC	Prasterona	2209007	26344SI	20
Fagron	Prasterona	22E25-F01-382686	26408SI[†]	20

- 201 284 spectra from a total of 4026 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 264 spectra from 67 *Apo-Ident* customers from 128 batches from the substance/substance group *Prasterona*.
- Among them are spectra of independent samples from 125 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prasterona	2206014-01	1
	Prasterona	22A17-F01-381261	1
	Prasterona	22E25-F01-382686	1
	Prasterona	2301031	1
	Prasterona	2301031-01	1
	Prasterona	2301032-01	2
	Prasterona	2301032-02	5
	Prasterona	2311028-01	1
	Prasterona	23K03-B04-231723	1
	Prasterona	23L01-B05-231787	1
	Prasterona	23L01-B05-238894	1
Audor Pharma	Prasterona	10050051/1P	1
Audor Pharma	Prasterona	AP11040002P	2
Audor Pharma	Prasterona	AP5103540P	1
Audor Pharma	Prasterona	APTDHAC17003-MD	3
Audor Pharma	Prasterona	APZDHA16003-M	1
Audor Pharma	Prasterona	APZDHAC17003-MD	3
Caelo	Prasterona	1412028-01	1
Caelo	Prasterona	15A15-B40-307323	1
Caelo	Prasterona	16B19-B04-318665	1
Caelo	Prasterona	16I02-B02-326485	1
Caelo	Prasterona	16l02-B02-326485	2
EuRho/Gehe	Prasterona	2005007-01	1
EuRho/Noweda	Prasterona	2101011-02	1
EuRho	Prasterona	1311002-01	1
Euro OTC	Prasterona	1306021-01	3
Euro OTC	Prasterona	1311002-01	2
Euro OTC	Prasterona	1401040-01	1
Euro OTC	Prasterona	1409004-01	4
Euro OTC	Prasterona	1412028	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prasterona	1412028-01	4
Euro OTC	Prasterona	1506011-01	4
Euro OTC	Prasterona	1602018-01	5
Euro OTC	Prasterona	1602018-02	2
Euro OTC	Prasterona	1702025	3
Euro OTC	Prasterona	170202501	1
Euro OTC	Prasterona	1702025-01	7
Euro OTC	Prasterona	1704012-01	1
Euro OTC	Prasterona	18050118-01	1
Euro OTC	Prasterona	1805018-01	4
Euro OTC	Prasterona	1809009-01	1
Euro OTC	Prasterona	1809009-03	6
Euro OTC	Prasterona	180901001	1
Euro OTC	Prasterona	1809010-01	4
Euro OTC	Prasterona	1901030-01	1
Euro OTC	Prasterona	1901030-02	1
Euro OTC	Prasterona	190103101	1
Euro OTC	Prasterona	1901031-01	3
Euro OTC	Prasterona	1901031-02	1
Euro OTC	Prasterona	1910025-01	3
Euro OTC	Prasterona	2001038-01	6
Euro OTC	Prasterona	200500701	1
Euro OTC	Prasterona	2005007-01	4
Euro OTC	Prasterona	2005008-01	11
Euro OTC	Prasterona	201101	2
Euro OTC	Prasterona	2081302	1
Euro OTC	Prasterona	2101011-02	7
Euro OTC	Prasterona	2101011-03	6
Euro OTC	Prasterona	2102004-02	2
Euro OTC	Prasterona	2102004-03	4
Euro OTC	Prasterona	2102004-04	1
Euro OTC	Prasterona	220103801	1
Euro OTC	Prasterona	2201038-01	7
Euro OTC	Prasterona	22021306	1
Euro OTC	Prasterona	2203004-01	1
Euro OTC	Prasterona	2206014-01	1
Euro OTC	Prasterona	220900701	1
Euro OTC	Prasterona	2209007-01	1
Euro OTC	Prasterona	23021711	1
Euro OTC	Prasterona	26031506	1
Euro OTC	Prasterona	30041509	1
Euro OTC	Prasterona	4091511	1
Euro OTC	Prasterona	5101849	1
Euro OTC	Prasterona	9215-4/09	1
Euro OTC	Prasterona	DHEA150801-1	1
Euro OTC	Prasterona	T03-04/1412028-01	1
Euro OTC	Prasterona	XPC0263	1
Euro OTC	Prasterona	ZDHAC18002	1
Euro/AHD	Prasterona	2005007-01	3
Euro/AHD	Prasterona	2102004-04	1
Fagron	Prasterona	12C26-N09	1
Fagron	Prasterona	12G04-N19	2
Fagron	Prasterona	12K30-N06	3
Fagron	Prasterona	13J10-B02	1
Fagron	Prasterona	13J10-B02-287177	1
Fagron	Prasterona	1421-B03-300211	1
Fagron	Prasterona	14C18-B02	1
Fagron	Prasterona	14c18b02293602	1
Fagron	Prasterona	14C18-B02-293602	1
Fagron	Prasterona	14C18-B02-293606	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prasterona	14C18-Bo2-293603	1
Fagron	Prasterona	14h12b05-297723	1
Fagron	Prasterona	14H12-B05-297727	2
Fagron	Prasterona	15A15-B40-307323	1
Fagron	Prasterona	15G14-B07-310827	1
Fagron	Prasterona	15I18-B09-316798	1
Fagron	Prasterona	16B19-B04-318665	2
Fagron	Prasterona	16B19-B04-322246	2
Fagron	Prasterona	16IO2-B02-326485	2
Fagron	Prasterona	16J26-B03-327602	1
Fagron	Prasterona	16L13-B01-332104	1
Fagron	Prasterona	17D11-B10-336395	1
Fagron	Prasterona	18B02-B02-345147	1
Fagron	Prasterona	18B13-B09_346424	1
Fagron	Prasterona	18C12	1
Fagron	Prasterona	18E15-B03-350802	2
Fagron	Prasterona	19061304	1
Fagron	Prasterona	19G10-B02-365017	2
Fagron	Prasterona	19G10-B02-365018	1
Fagron	Prasterona	19G10-B02-365154	2
Fagron	Prasterona	19G10-B02-365155	1
Fagron	Prasterona	20123-F03-374815	2
Fagron	Prasterona	20C25-U03-005782	1
Fagron	Prasterona	20I23-F03-374815	1
Fagron	Prasterona	20l23-F03-374815	1
Fagron	Prasterona	21G13-F03-380169	6
Fagron	Prasterona	21G13-F03-380169	1
Fagron	Prasterona	22A17-F01-381262	1
Fagron	Prasterona	22H22-B04-223769	1
Fagron	Prasterona	22K21-B05-225380	1
Fagron	Prasterona	27071705	1
Fagron	Prasterona	7013260004	1
Fagron	Prasterona	701326-0005	1
Fagron	Prasterona	C04-140804(M)	1
Fagron	Prasterona	DHEA160802	1
Fagron	Prasterona	DHEA190504	2
Fagron	Prasterona	DHEAA150401-1	1
Fagron	Prasterona	DHEAH200604W	2
Fagron	Prasterona	F02-3779709	1
Fargon	Prasterona	16B19-B04-318665	1
Fragon	Prasterona	12G04-N19	1
Gall Pharma	Prasterona	16/02-B02	1
Gehe	Prasterona	2005007-01	2
Gehe	Prasterona	2102004-02	2
Haihang Industry	Prasterona	20130816	4
Haihang	Prasterona	20130507	1
Jacoby Gatt-Koller	Prasterona	20J02359	1
Kögl	Prasterona	1803108	1
Nachprüfung	Prasterona	120022	1
NWM Shandong Northwe…	Prasterona	PST151207	1
Ph.Eur/AHD	Prasterona	1809009-03	1
Phönix	Prasterona	2102004-04	4
PROQUINA	Prasterona	1602018_02	1
Sanacorp	Prasterona	1805018-01	1
Sanacorp	Prasterona	2203004-01	1

- 235 803 spectra from 1515 *Apo-Ident* customers from a total of 49 131 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prasterona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prasterona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	909	0	152 053
Type B	0	800	0	201 284
Type C	0	264	0	235 803

The substance/substance group *Prasterona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3399 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20703	20703	0,00	149,79
20960	20960	0,00	149,04
21824	21824	0,00	143,19
21917	25091	26,60	143,38
22506	22506	0,00	152,62
23389	23389	0,00	108,92
23695	23695	0,00	122,12
23865	23695	43,72	137,04
23868	23868	0,00	111,98
23893	23893	0,00	134,02
23931	23931	0,00	138,91
24323	24323	0,00	138,36
24412	23893	6,84	133,77

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24430	24430	0,00	116,37
24853	24853	0,00	140,32
24966	24966	0,00	148,99
24967	24967	0,00	147,68
25091	25091	0,00	146,98
25537	25537	0,00	149,88
25568	25568	0,00	148,40
26408	25091	15,42	150,52
26513	26513	0,00	145,96

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Praziquantel**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24840-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Praziquantel; Praziquantelum

Special notes

When selecting the *Praziquantel* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Praziquantel	3	1	0

Second-stage model

For differentiation of the substance/substance group *Praziquantel* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Praziquantel* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ofloxacino	82,57	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Praziquantel* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Praziquantel*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Praziquantel	2205031	26185	40	20220620*
Euro OTC	Praziquantel	2205031	26185SI	20	20220620*
Euro OTC	Praziquantel	2401015	27159	30	20240227*
Euro OTC	Praziquantel	2402035	27162	40	20240313*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 130 spectra of 4 reference samples from the substance/substance group *Praziquantel*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 832 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Praziquantel*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Praziquantel	1908004	24840	40
Euro OTC	Praziquantel	2401015	27159SI†	20
Euro OTC	Praziquantel	2402035	27162SI†	20

- 202 004 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Praziquantel*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Praziquantel* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Praziquantel* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	130	0	152 832
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Praziquantel* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26185	26185	0,00	104,62
27159	27159	0,00	104,31
27162	27162	0,00	102,70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednicarbato**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20196-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednicarbato; Prednicarbatum

Special notes

When selecting the *Prednicarbato* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednicarbato	13	18	495

Second-stage model

For differentiation of the substance/substance group *Prednicarbato* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednicarbato* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	48,83	–
Ciclosporina	111,03	–
⋮	⋮	⋮
Cloridrato de oxibutinina	>50	63,41
Levocarnitina	>50	146,11
Capsaicina	>50	149,61
Citrato de sódio	>50	160,35
Acetato de ciproterona	>50	191,37
Tetracaína	>50	217,19
Acetato de noretisterona	>50	224,58
Cloridrato de amitriptilina	>50	328,16
Cloridrato de quinina di-hidratado	>50	411,25
Heparina sódica	>50	428,04
Alfaestradiol	>50	529,52
Piridoxal-5-fosfato	>50	584,42
Valina	>50	610,65
Metoxisaleno	>50	627,94
Cloridrato de ciprofloxacina	>50	635,05
Sacarose	>50	1932,95
Amifampridina	>50	2013,98
Triclosan	>50	2054,82

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednicarbato* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednicarbato*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednicarbato	13119402	20832	60	1501576
Caelo	Prednicarbato	13119402	20833	60	20130517
Caelo	Prednicarbato	13119402	20833SI	30	20130517
Caelo	Prednicarbato	13372404	21368	50	AR-15-FG-007941-02
Caelo	Prednicarbato	13372404	21369	49	20131119
Caelo	Prednicarbato	13372404	21369SI	33	20131119
Euro OTC	Prednicarbato	1302033-02	21610	60	1509286
Euro OTC	Prednicarbato	1507011	21858	60	20150730*
Euro OTC	Prednicarbato	1601058	22366	45	20160223*
Euro OTC	Prednicarbato	1601058	22366SI	31	20160223*
Euro OTC	Prednicarbato	2001031	25119	40	20200331*
Euro OTC	Prednicarbato	2009018	25401	40	20200930*
Euro OTC	Prednicarbato	2103017	25609	40	20210408*
Euro OTC	Prednicarbato	2103017	25609SI	38	20210408*
Euro OTC	Prednicarbato	2204014	26084	40	20220511*
Euro OTC	Prednicarbato	2405019	27277	40	20240704*
Euro OTC	Prednicarbato	2405019	27277SI	30	20240704*
Fagron	Prednicarbato	12D27-N04	20700	40	20120509
Fagron	Prednicarbato	12D27-N04	20700SI	48	20120509
Fagron	Prednicarbato	14A27-B02-291256	21572	60	AR-16-FG-011442-01
Fagron	Prednicarbato	22F03-B02-223103	26393	40	20220930
Fagron	Prednicarbato	22F03-B02-223103	26393SI	30	20220930

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 964 spectra of 22 reference samples from the substance/substance group *Prednicarbato*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 151 998 spectra from a total of 2829 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1297 spectra of 41 reference samples from the substance/substance group *Prednicarbato*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednicarbato	160874	22447	60
Caelo	Prednicarbato	170138	23040	40
Caelo	Prednicarbato	173156	23845	40
Caelo	Prednicarbato	172204	23848	40
Caelo	Prednicarbato	21001161001	25928	40
Caelo	Prednicarbato	22000755	26130	40
Caelo	Prednicarbato	23001025	26847	40
Caelo	Prednicarbato	23001026	26848	40
Euro OTC	Prednicarbato	1605001	22558	30
Euro OTC	Prednicarbato	1607012	22703	40
Euro OTC	Prednicarbato	1609022	22860	40
Euro OTC	Prednicarbato	1707022	23540	40
Euro OTC	Prednicarbato	1801013	23887	40
Euro OTC	Prednicarbato	1805005	24134	40
Euro OTC	Prednicarbato	1809015	24320	40
Euro OTC	Prednicarbato	1903023	24633	40
Euro OTC	Prednicarbato	2304020	26922	40
Euro OTC	Prednicarbato	2411003	27458	30
Caelo	Prednicarbato	160874	22447SI	30
Caelo	Prednicarbato	170138	23040SI	20
Caelo	Prednicarbato	173156	23845SI	20
Caelo	Prednicarbato	172204	23848SI	20
Caelo	Prednicarbato	21001161001	25928SI	36
Caelo	Prednicarbato	22000755	26130SI	30
Caelo	Prednicarbato	23001025	26847SI	30
Caelo	Prednicarbato	23001026	26848SI	30
Euro OTC	Prednicarbato	1507011	21858SI†	15
Euro OTC	Prednicarbato	1605001	22558SI	25
Euro OTC	Prednicarbato	1607012	22703SI	28
Euro OTC	Prednicarbato	1609022	22860SI	27
Euro OTC	Prednicarbato	1707022	23540SI	19
Euro OTC	Prednicarbato	1801013	23887SI	20
Euro OTC	Prednicarbato	1805005	24134SI	20
Euro OTC	Prednicarbato	1809015	24320SI	20
Euro OTC	Prednicarbato	1903023	24633SI	32
Euro OTC	Prednicarbato	2001031	25119SI†	27
Euro OTC	Prednicarbato	2009018	25401SI†	25
Euro OTC	Prednicarbato	2204014	26084SI†	10
Euro OTC	Prednicarbato	2304020	26922SI	37
Euro OTC	Prednicarbato	2411003	27458SI	20
Fagron	Prednicarbato	14A27-B02-291256	21572SI†	36

- 200 787 spectra from a total of 4022 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

provided by the customer regarding manufacturer and batch number.

- 3979 spectra from 1071 *Apo-Ident* customers from 515 batches from the substance/substance group *Prednicarbato*.
- Among them are spectra of independent samples from 493 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednicarbato	2001031-01	1
	Prednicarbato	21000991002	1
	Prednicarbato	21001161004	1
	Prednicarbato	21001161006	1
	Prednicarbato	21001161011	1
	Prednicarbato	2103017-01	3
	Prednicarbato	21F07-B17-216553	1
	Prednicarbato	22000755001	6
	Prednicarbato	22000755002	2
	Prednicarbato	22000755003	1
	Prednicarbato	22000755005	3
	Prednicarbato	22000755007	5
	Prednicarbato	22000755008	5
	Prednicarbato	22000755009	13
	Prednicarbato	22000755010	6
	Prednicarbato	2200755002	2
	Prednicarbato	220401401	2
	Prednicarbato	2204014-01	13
	Prednicarbato	2204014-02	1
	Prednicarbato	22F03-B02_223103	1
	Prednicarbato	22F03-B02-218938	1
	Prednicarbato	22F03-B02-223102	5
	Prednicarbato	22F03-B02-223103	2
	Prednicarbato	22F03-B02-223104	1
	Prednicarbato	22F03-B02-2277918	1
	Prednicarbato	22F03-B02-227918	4
	Prednicarbato	22F03-B02-227919	2
	Prednicarbato	22F03-B02-232393	2
	Prednicarbato	23001025003	3
	Prednicarbato	23001026001	26
	Prednicarbato	23001026002	23
	Prednicarbato	23001026003	3
	Prednicarbato	23003318001	1
	Prednicarbato	2304020_01	1
	Prednicarbato	2304020-01	15
	Prednicarbato	2304040-01	1
	Prednicarbato	23H24-B06-232394	2
	Prednicarbato	B06-2323904	1
19Caesar & Loretz GmbH	Prednicarbato	22000755001	1
AEP	Prednicarbato	19E14-B01-191430	3
AEP	Prednicarbato	21000991003	1
AEP	Prednicarbato	22000755003	1
AHC	Prednicarbato	20000609004	1
AHC	Prednicarbato	20000609009	1
AHC	Prednicarbato	20003660005	2
AHC	Prednicarbato	2009018-01	1
AHD	Prednicarbato	17220408	1
AHD	Prednicarbato	1801013-01	1
AHD	Prednicarbato	1809015-01	1
AHD	Prednicarbato	21001161001	1
AHD	Prednicarbato	21001161006	1
AHD	Prednicarbato	21K24-B03-213699	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Prednicarbato	2204014-01	1
AHD	Prednicarbato	23001026001	1
AHD	Prednicarbato	23001026003	1
AHD	Prednicarbato	23003318001	1
AHD	Prednicarbato	2304020-01	1
AHL	Prednicarbato	16087408	2
Alliance Healthcare	Prednicarbato	21001161010	1
Alliance Healthcare	Prednicarbato	22000755002	1
Alliance Healthcare	Prednicarbato	22000755003	1
Alliance Healthcare	Prednicarbato	2204014-01	1
Alliance	Prednicarbato	22000755002	1
Alliance	Prednicarbato	22000755010	1
Anzag	Prednicarbato	17220408	1
Apo-ident/Phoenix	Prednicarbato	1903023-01	1
apo-ident	Prednicarbato	1607012-01	1
apomix	Prednicarbato	13372410	2
apomix	Prednicarbato	1609022-01	2
Bombastus	Prednicarbato	15446306	1
Bombastus	Prednicarbato	17220408	1
Bombastus	Prednicarbato	17315605	1
Caelo	Prednicarbato		3
Caelo	Prednicarbato	118194105	1
Caelo	Prednicarbato	11L23-N07	2
Caelo	Prednicarbato	12(20000609009)	1
Caelo	Prednicarbato	121223613	1
Caelo	Prednicarbato	12123610	1
Caelo	Prednicarbato	1213608	1
Caelo	Prednicarbato	1220218/17220407	1
Caelo	Prednicarbato	12383301	1
Caelo	Prednicarbato	12383309	1
Caelo	Prednicarbato	13(20003660005)	1
Caelo	Prednicarbato	13/23-N04	1
Caelo	Prednicarbato	13119401	1
Caelo	Prednicarbato	13119402	2
Caelo	Prednicarbato	13224401	5
Caelo	Prednicarbato	13224406	2
Caelo	Prednicarbato	13372403	11
Caelo	Prednicarbato	13372408	1
Caelo	Prednicarbato	13372410	6
Caelo	Prednicarbato	13372411	1
Caelo	Prednicarbato	13372419	6
Caelo	Prednicarbato	14(20003660008)	1
Caelo	Prednicarbato	14A27-B02-295796	1
Caelo	Prednicarbato	14A27-B02-295797	1
Caelo	Prednicarbato	14J16-B06	3
Caelo	Prednicarbato	15(21000991002)	1
Caelo	Prednicarbato	1507011-01	1
Caelo	Prednicarbato	1517E-03595	1
Caelo	Prednicarbato	15181403	13
Caelo	Prednicarbato	15181404	3
Caelo	Prednicarbato	15181408	1
Caelo	Prednicarbato	15181409	4
Caelo	Prednicarbato	15181411	2
Caelo	Prednicarbato	15446301	22
Caelo	Prednicarbato	15446302	13
Caelo	Prednicarbato	15446303	3
Caelo	Prednicarbato	1544630306	1
Caelo	Prednicarbato	15446304	1
Caelo	Prednicarbato	15446305	6
Caelo	Prednicarbato	15446306	13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbato	15D15-B03	1
Caelo	Prednicarbato	15D15-B03-308161	1
Caelo	Prednicarbato	15D15-B03-310847	2
Caelo	Prednicarbato	15G10-B02-314082	3
Caelo	Prednicarbato	15J22-B04-318528	1
Caelo	Prednicarbato	15J22-B-321005	1
Caelo	Prednicarbato	1601058-01	1
Caelo	Prednicarbato	160500	1
Caelo	Prednicarbato	1605001	1
Caelo	Prednicarbato	160701201	1
Caelo	Prednicarbato	1607012-01	2
Caelo	Prednicarbato	1608710	1
Caelo	Prednicarbato	16087401	13
Caelo	Prednicarbato	16087408	20
Caelo	Prednicarbato	16087410	22
Caelo	Prednicarbato	16087411	3
Caelo	Prednicarbato	16087412	6
Caelo	Prednicarbato	1609022-01	3
Caelo	Prednicarbato	168087410	1
Caelo	Prednicarbato	16987410	1
Caelo	Prednicarbato	16A18-B01-322732	1
Caelo	Prednicarbato	16A18-B01-322733	2
Caelo	Prednicarbato	16E12-B01	1
Caelo	Prednicarbato	16E12-B01-325758	1
Caelo	Prednicarbato	16J27-B01	1
Caelo	Prednicarbato	16J27-B01-330976	3
Caelo	Prednicarbato	16J27-B01-330977	1
Caelo	Prednicarbato	16J27-B01-332958	1
Caelo	Prednicarbato	17013804	14
Caelo	Prednicarbato	17013805	11
Caelo	Prednicarbato	17014001	3
Caelo	Prednicarbato	17014003	28
Caelo	Prednicarbato	17014005	20
Caelo	Prednicarbato	17014006	2
Caelo	Prednicarbato	1704003	1
Caelo	Prednicarbato	1704005	1
Caelo	Prednicarbato	1707022-01	3
Caelo	Prednicarbato	17220401	6
Caelo	Prednicarbato	17220406	4
Caelo	Prednicarbato	17220407	46
Caelo	Prednicarbato	1722040716J27-B01-33	1
Caelo	Prednicarbato	172204075515	1
Caelo	Prednicarbato	17220408	48
Caelo	Prednicarbato	17220410	2
Caelo	Prednicarbato	1722401	1
Caelo	Prednicarbato	173156	1
Caelo	Prednicarbato	17315603	7
Caelo	Prednicarbato	17315604	38
Caelo	Prednicarbato	17315605	28
Caelo	Prednicarbato	17315606	1
Caelo	Prednicarbato	17315607	2
Caelo	Prednicarbato	17315609	46
Caelo	Prednicarbato	17315611	3
Caelo	Prednicarbato	177220407	1
Caelo	Prednicarbato	17C27-B01-339079	1
Caelo	Prednicarbato	17J04-B05-343934	1
Caelo	Prednicarbato	17j04B05346113	1
Caelo	Prednicarbato	17J04-B05-346113	1
Caelo	Prednicarbato	180101301	1
Caelo	Prednicarbato	1801013-01	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbato	1805005-01	1
Caelo	Prednicarbato	1814112	1
Caelo	Prednicarbato	1819104	1
Caelo	Prednicarbato	18194101	1
Caelo	Prednicarbato	18194103	12
Caelo	Prednicarbato	18194104	61
Caelo	Prednicarbato	18194105	80
Caelo	Prednicarbato	18194112	9
Caelo	Prednicarbato	18194115	48
Caelo	Prednicarbato	18194116	5
Caelo	Prednicarbato	18194117	21
Caelo	Prednicarbato	18194194	1
Caelo	Prednicarbato	18197115	1
Caelo	Prednicarbato	18294103	1
Caelo	Prednicarbato	18B27-B01-350264	2
Caelo	Prednicarbato	18E14-B03-352560	2
Caelo	Prednicarbato	18E14-B03-355726	1
Caelo	Prednicarbato	18E14-B03-355727	1
Caelo	Prednicarbato	19051601	57
Caelo	Prednicarbato	19051602	47
Caelo	Prednicarbato	1905-1602	1
Caelo	Prednicarbato	19051603	1
Caelo	Prednicarbato	19051604	9
Caelo	Prednicarbato	191122608	1
Caelo	Prednicarbato	19122602	18
Caelo	Prednicarbato	19122604	53
Caelo	Prednicarbato	19122608	53
Caelo	Prednicarbato	1922604	2
Caelo	Prednicarbato	1922608	1
Caelo	Prednicarbato	19G09-B01-194722	2
Caelo	Prednicarbato	2(18194104)	1
Caelo	Prednicarbato	200000609004	2
Caelo	Prednicarbato	20000360007	1
Caelo	Prednicarbato	200003660006	2
Caelo	Prednicarbato	200003660007	3
Caelo	Prednicarbato	20000609001	14
Caelo	Prednicarbato	20000609003	1
Caelo	Prednicarbato	20000609004	57
Caelo	Prednicarbato	20000609006	12
Caelo	Prednicarbato	20000609008	1
Caelo	Prednicarbato	20000609009	37
Caelo	Prednicarbato	2000060904	1
Caelo	Prednicarbato	20000609606	1
Caelo	Prednicarbato	2000360009	1
Caelo	Prednicarbato	20003660002	1
Caelo	Prednicarbato	20003660004	10
Caelo	Prednicarbato	20003660005	12
Caelo	Prednicarbato	20003660006	22
Caelo	Prednicarbato	20003660007	30
Caelo	Prednicarbato	200036600078	1
Caelo	Prednicarbato	20003660008	34
Caelo	Prednicarbato	20003660008mul	1
Caelo	Prednicarbato	20003660009	31
Caelo	Prednicarbato	2000366005	1
Caelo	Prednicarbato	2000366006	1
Caelo	Prednicarbato	2000366007	3
Caelo	Prednicarbato	2000366008	3
Caelo	Prednicarbato	2000366009	1
Caelo	Prednicarbato	200036660008	1
Caelo	Prednicarbato	20006069006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbato	2000609004	1
Caelo	Prednicarbato	2001031-01	5
Caelo	Prednicarbato	2003660007	1
Caelo	Prednicarbato	2003660008	2
Caelo	Prednicarbato	2003666009	1
Caelo	Prednicarbato	2009018-01	5
Caelo	Prednicarbato	2009018-02	1
Caelo	Prednicarbato	201372	1
Caelo	Prednicarbato	2018821009912	1
Caelo	Prednicarbato	20A21-B12	1
Caelo	Prednicarbato	2100091003	2
Caelo	Prednicarbato	21000991001	2
Caelo	Prednicarbato	21000991002	45
Caelo	Prednicarbato	21000991003	34
Caelo	Prednicarbato	21000991004	2
Caelo	Prednicarbato	21000991005	8
Caelo	Prednicarbato	2100116007	2
Caelo	Prednicarbato	21001161001	48
Caelo	Prednicarbato	21001161003	2
Caelo	Prednicarbato	21001161004	3
Caelo	Prednicarbato	21001161006	31
Caelo	Prednicarbato	21001161007	28
Caelo	Prednicarbato	21001161008	4
Caelo	Prednicarbato	21001161010	17
Caelo	Prednicarbato	21001161011	20
Caelo	Prednicarbato	21001161013	5
Caelo	Prednicarbato	2100161001	3
Caelo	Prednicarbato	2100161006	1
Caelo	Prednicarbato	2100161007	4
Caelo	Prednicarbato	2100991003	3
Caelo	Prednicarbato	2101161011	1
Caelo	Prednicarbato	2103017-01	2
Caelo	Prednicarbato	210906(21000991002)	1
Caelo	Prednicarbato	211001161011	1
Caelo	Prednicarbato	211007	1
Caelo	Prednicarbato	21990000022000	1
Caelo	Prednicarbato	21F07-817-216553	1
Caelo	Prednicarbato	21F07-B17-216554	1
Caelo	Prednicarbato	22000755001	13
Caelo	Prednicarbato	22000755002	10
Caelo	Prednicarbato	22000755003	15
Caelo	Prednicarbato	22000755005	3
Caelo	Prednicarbato	22000755006	2
Caelo	Prednicarbato	22000755007	9
Caelo	Prednicarbato	22000755009	1
Caelo	Prednicarbato	2200075509	2
Caelo	Prednicarbato	220075507	1
Caelo	Prednicarbato	22007553003	1
Caelo	Prednicarbato	220516(21001161010)	1
Caelo	Prednicarbato	23001026001	4
Caelo	Prednicarbato	23051819	1
Caelo	Prednicarbato	23082013A	1
Caelo	Prednicarbato	2748	1
Caelo	Prednicarbato	2790	1
Caelo	Prednicarbato	2x21001161001	1
Caelo	Prednicarbato	3(19051602)	1
Caelo	Prednicarbato	3267	1
Caelo	Prednicarbato	3272	1
Caelo	Prednicarbato	3302	1
Caelo	Prednicarbato	3438	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbato	6090092	1
Caelo	Prednicarbato	718A-03595	1
Caelo	Prednicarbato	9764897	1
Caelo	Prednicarbato	C0333/1111070	2
Caelo	Prednicarbato	PNC101/0720	1
Caeol/Noweda	Prednicarbato	16A18-B01-322732	1
Caeol/Noweda	Prednicarbato	17315609	1
Caeol/Phornix	Prednicarbato	17315604	1
Caersar & Loretz	Prednicarbato	21000991002	1
Caesar & Lorenz GmbH	Prednicarbato	19051601	1
Caesar & Lorenz GmbH	Prednicarbato	19051602	1
Caesar & Loretz GmbH...	Prednicarbato	19051601	1
Caesar & Loretz GmbH...	Prednicarbato	21001161004	1
Caesar & Loretz GmbH...	Prednicarbato	21001161007	3
Caesar & Loretz GmbH...	Prednicarbato	18194112	1
Caesar & Loretz GmbH...	Prednicarbato	21000991002	1
Caesar & Loretz GmbH...	Prednicarbato	20003660009	1
Caesar & Loretz GmbH...	Prednicarbato	20000609009	1
Caesar & Loretz GmbH/ AHD	Prednicarbato	22000755003	1
Caesar & Loretz GmbH...	Prednicarbato	20000609004	1
Caesar & Loretz GmbH...	Prednicarbato	21001161007	1
Caesar & Loretz GmbH...	Prednicarbato	21001161010	1
Caesar & Loretz GmbH...	Prednicarbato	21001161011	1
Caesar & Loretz GmbH/AHD	Prednicarbato	20000609004	1
Caesar & Loretz GmbH/AHD	Prednicarbato	21001161010	1
Caesar & Loretz GmbH/E	Prednicarbato	21000991003	1
Caesar & Loretz GmbH...	Prednicarbato	1203584	1
Caesar & Loretz GmbH...	Prednicarbato	19122608	1
Caesar & Loretz GmbH...	Prednicarbato	21001161007	1
Caesar & Loretz GmbH...	Prednicarbato	B12-1975501	1
Caesar & Loretz GmbH/G	Prednicarbato	20003660009	1
Caesar & Loretz GmbH/G	Prednicarbato	21001161006	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	18194115	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	191226	1
Caesar & Loretz GmbH/GEHE	Prednicarbato	19122602	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	19122604	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	20000609004	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	20000609006	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	20000609009	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	21000991003	1
Caesar & Loretz GmbH/Gehe	Prednicarbato	21001161006	1
Caesar & Loretz GmbH...	Prednicarbato	21000991002	1
Caesar & Loretz GmbH...	Prednicarbato	21001161006	1
Caesar & Loretz GmbH...	Prednicarbato	18194117	1
Caesar & Loretz GmbH...	Prednicarbato	20003660009	1
Caesar & Loretz GmbH...	Prednicarbato	21001161006	2
Caesar & Loretz GmbH...	Prednicarbato	19122604	1
Caesar & Loretz GmbH...	Prednicarbato	20000609004	1
Caesar & Loretz GmbH...	Prednicarbato	20003660004	1
Caesar & Loretz GmbH...	Prednicarbato	21001161007	1
Caesar & Loretz GmbH...	Prednicarbato	21001161011	1
Caesar & Loretz GmbH...	Prednicarbato	19051602	1
Caesar & Loretz GmbH...	Prednicarbato	20003660005	1
Caesar & Loretz GmbH...	Prednicarbato	21000991002	1
Caesar & Loretz GmbH...	Prednicarbato	21001161001	6
Caesar & Loretz GmbH...	Prednicarbato	21001161006	1
Caesar & Loretz GmbH...	Prednicarbato	19122602	1
Caesar & Loretz GmbH...	Prednicarbato	20000609009	1
Caesar & Loretz GmbH...	Prednicarbato	20003660008	1
Caesar & Loretz GmbH/sa	Prednicarbato	22000755001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Prednicarbato	19122604	1
Caesar & Loretz GmbH...	Prednicarbato	20003660007	1
Caesar & Loretz GmbH...	Prednicarbato	21001161001	1
Caesar & Loretz GmbH...	Prednicarbato	AP221018-02	1
Caesar & Loretz GmbH	Prednicarbato	16087410	1
Caesar & Loretz GmbH	Prednicarbato	18194103	1
Caesar & Loretz GmbH	Prednicarbato	18194104	1
Caesar & Loretz GmbH	Prednicarbato	18194105	12
Caesar & Loretz GmbH	Prednicarbato	18194115	10
Caesar & Loretz GmbH	Prednicarbato	18194117	1
Caesar & Loretz GmbH	Prednicarbato	19051601	1
Caesar & Loretz GmbH	Prednicarbato	19051602	10
Caesar & Loretz GmbH	Prednicarbato	19122602	4
Caesar & Loretz GmbH	Prednicarbato	19122604	6
Caesar & Loretz GmbH	Prednicarbato	19122608	7
Caesar & Loretz GmbH	Prednicarbato	20000609004	16
Caesar & Loretz GmbH	Prednicarbato	20000609006	6
Caesar & Loretz GmbH	Prednicarbato	20000609009	14
Caesar & Loretz GmbH	Prednicarbato	20003660004	5
Caesar & Loretz GmbH	Prednicarbato	20003660005	4
Caesar & Loretz GmbH	Prednicarbato	20003660006	5
Caesar & Loretz GmbH	Prednicarbato	20003660007	10
Caesar & Loretz GmbH	Prednicarbato	20003660008	13
Caesar & Loretz GmbH	Prednicarbato	20003660009	4
Caesar & Loretz GmbH	Prednicarbato	21000991002	8
Caesar & Loretz GmbH	Prednicarbato	21000991003	10
Caesar & Loretz GmbH	Prednicarbato	21000991005	8
Caesar & Loretz GmbH	Prednicarbato	21001161001	14
Caesar & Loretz GmbH	Prednicarbato	21001161004	3
Caesar & Loretz GmbH	Prednicarbato	21001161006	11
Caesar & Loretz GmbH	Prednicarbato	21001161007	10
Caesar & Loretz GmbH	Prednicarbato	21001161008	4
Caesar & Loretz GmbH	Prednicarbato	21001161010	6
Caesar & Loretz GmbH	Prednicarbato	21001161011	9
Caesar & Loretz GmbH	Prednicarbato	21001161013	2
Caesar & Loretz GmbH	Prednicarbato	21A11-B01-2035804	1
Caesar & Loretz GmbH	Prednicarbato	22000755001	5
Caesar & Loretz GmbH	Prednicarbato	22000755002	3
Caesar & Loretz GmbH	Prednicarbato	22000755003	6
Caesar & Loretz GmbH	Prednicarbato	22000755005	1
Caesar & Loretz GmbH	Prednicarbato	22000755007	7
Caesar & Loretz GmbH	Prednicarbato	22000755009	2
Caesar & Loretz GmbH	Prednicarbato	22000755010	1
Caesar & Loretz GmbH	Prednicarbato	23001026001	2
Caesar & Loretz GmbH	Prednicarbato	23001026002	1
Caesar & Loretz Hild...	Prednicarbato	19051602	2
Caesar & Loretz Hild...	Prednicarbato	20000609004	1
Caesar & Loretz Hilden	Prednicarbato	18194104	1
Caesar & Loretz Hilden	Prednicarbato	19122608	2
Caesar & Loretz Hilden	Prednicarbato	20000609009	2
Caesar & Loretz Hilden	Prednicarbato	2009018-01	1
Caesar & Loretz/Geil...	Prednicarbato	19051602	1
Caesar & Loretz/Noweda	Prednicarbato	20000609004	1
Caesar & Loretz/Noweda	Prednicarbato	20003660005	1
Caesar Loretz	Prednicarbato	20003660007	1
Caesar und Loretz GmbH	Prednicarbato	17220406	1
caesar&loretz GmbH,A...	Prednicarbato	16087408	1
Caesar&Loretz GmbH/ ...	Prednicarbato	19122604	1
Caesar&Loretz GmbH	Prednicarbato	20003660006	1
Caesar&Loretz GmbH	Prednicarbato	22000755003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
caesar&loretz,Phönix	Prednicarbato	15181411	1
caesar&loretz	Prednicarbato	18149103	1
Caesar/Ebert	Prednicarbato	18194105	1
Caleo/ Fiebig	Prednicarbato	17J04-B05-341872	1
Caleo/Krieger	Prednicarbato	21001161007	1
Cealo/GEHE	Prednicarbato	17315609	1
Cealo/Jenne	Prednicarbato	220306(21001161006)	1
Cealo/Phönix	Prednicarbato	20000609004	1
Cealo/Sanacorp	Prednicarbato	15546306	1
cealo	Prednicarbato	14J16-B06-303465	1
Celo	Prednicarbato	1687408	1
Defektur	Prednicarbato	12D27-N04	1
E und J, 22.07.2016	Prednicarbato	15446306	2
Eu Rho	Prednicarbato	2103017-01	1
Eurho / Alliance	Prednicarbato	2103017-01	2
EuRho / Noweda	Prednicarbato	1903023-01	4
EuRho/ AHD	Prednicarbato	1801013-01	1
EuRho/ AHD	Prednicarbato	1805005	1
EuRho/ NOWEDA	Prednicarbato	1903023-01	1
EuRho/ NOWEDA	Prednicarbato	2001031-01	1
EuRho/Gehe	Prednicarbato	1801013-01	2
eurho/gehe	Prednicarbato	2009018-01	1
EuRho/Noweda	Prednicarbato	1805005-01	1
EuRho/Noweda	Prednicarbato	200901801	1
Eurho/noweda	Prednicarbato	210301701	1
EuRho/Phoenix	Prednicarbato	2009018-01	1
EuRho/Phönix	Prednicarbato	1805005-01	2
EuRho/Phönix	Prednicarbato	2001031-01	1
EuRho	Prednicarbato	1801013-01	1
EuRho	Prednicarbato	2103017-01	1
Euro OCT / Krieger	Prednicarbato	2009018-01	6
Euro OTC	Prednicarbato		3
Euro OTC	Prednicarbato	1302033-01	1
Euro OTC	Prednicarbato	1302033-02	3
Euro OTC	Prednicarbato	13224402	1
Euro OTC	Prednicarbato	13372403	1
Euro OTC	Prednicarbato	1501033-01	2
Euro OTC	Prednicarbato	1501033-02	4
Euro OTC	Prednicarbato	1507011-01	2
Euro OTC	Prednicarbato	1507011-02	4
Euro OTC	Prednicarbato	1601058-01	5
Euro OTC	Prednicarbato	1605001	1
Euro OTC	Prednicarbato	1605001-01	10
Euro OTC	Prednicarbato	1607012-01	11
Euro OTC	Prednicarbato	1609011-01	1
Euro OTC	Prednicarbato	160902	1
Euro OTC	Prednicarbato	160902201	3
Euro OTC	Prednicarbato	1609022-01	21
Euro OTC	Prednicarbato	170702201	1
Euro OTC	Prednicarbato	1707022-01	40
Euro OTC	Prednicarbato	1707022201	1
Euro OTC	Prednicarbato	17220408	2
Euro OTC	Prednicarbato	1801013	1
Euro OTC	Prednicarbato	180101301	1
Euro OTC	Prednicarbato	1801013-01	33
Euro OTC	Prednicarbato	1805001-01	2
Euro OTC	Prednicarbato	180500501	1
Euro OTC	Prednicarbato	1805005-01	27
Euro OTC	Prednicarbato	1805005-02	2
Euro OTC	Prednicarbato	1809015001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prednicarbato	180901501	4
Euro OTC	Prednicarbato	1809015-01	37
Euro OTC	Prednicarbato	1809015-02	2
Euro OTC	Prednicarbato	18E14-B03-355726	1
Euro OTC	Prednicarbato	190023-01	1
Euro OTC	Prednicarbato	1902012-01	1
Euro OTC	Prednicarbato	1903023	2
Euro OTC	Prednicarbato	190302301	3
Euro OTC	Prednicarbato	1903023-01	76
Euro OTC	Prednicarbato	1903023-02	1
Euro OTC	Prednicarbato	19032023-01	1
Euro OTC	Prednicarbato	190741607	1
Euro OTC	Prednicarbato	20001031-01	1
Euro OTC	Prednicarbato	20009018-01	1
Euro OTC	Prednicarbato	200103101	5
Euro OTC	Prednicarbato	2001031-01	83
Euro OTC	Prednicarbato	20090018-01	1
Euro OTC	Prednicarbato	200901-01	1
Euro OTC	Prednicarbato	200901801	3
Euro OTC	Prednicarbato	2009018-01	149
Euro OTC	Prednicarbato	2009018-012x	1
Euro OTC	Prednicarbato	2009018-02	22
Euro OTC	Prednicarbato	200918-01	2
Euro OTC	Prednicarbato	209018-01	1
Euro OTC	Prednicarbato	210301701	3
Euro OTC	Prednicarbato	2103017-01	68
Euro OTC	Prednicarbato	2103017-02	4
Euro OTC	Prednicarbato	210317-01	1
Euro OTC	Prednicarbato	2204014_01	1
Euro OTC	Prednicarbato	2204014-01	16
Euro OTC	Prednicarbato	220414-01	1
Euro OTC	Prednicarbato	23001026001	1
Euro OTC	Prednicarbato	2304020-01	1
Euro OTC	Prednicarbato	3103017-01	1
Euro OTC	Prednicarbato	B01-2035804	1
Euro OTC	Prednicarbato	B05-2016409	1
Euro OTC	Prednicarbato	PNC101/0720	1
Euro Pharma/Gehe	Prednicarbato	1801013-01	1
Euro/Gehe	Prednicarbato	1609022-01	1
Euro/Gehe	Prednicarbato	1805005-01	1
Euro/Phönix	Prednicarbato	1607012-01	1
Euro/Phönix	Prednicarbato	1809015-01	2
Euro/Phönix	Prednicarbato	1903023-01	1
Euro/Phönix	Prednicarbato	2204014-01	1
Euro	Prednicarbato	1507011-01	1
EuRoh/ Gehe	Prednicarbato	18E14-B03-355726	2
Fagr	Prednicarbato	18E14-B03-352560	2
Fagro/Gehe	Prednicarbato	15D15-B03-308161	1
Fagro/Sanacorp	Prednicarbato	19G09-B01-194724	1
Fagron	Prednicarbato		1
Fagron	Prednicarbato	10J04-N10	1
Fagron	Prednicarbato	11L23-N07	4
Fagron	Prednicarbato	12B20-N06	3
Fagron	Prednicarbato	12D27-N04	3
Fagron	Prednicarbato	12H20-N07	1
Fagron	Prednicarbato	13/23-N04	3
Fagron	Prednicarbato	13372408	1
Fagron	Prednicarbato	13C25-N02	1
Fagron	Prednicarbato	13C25-N06	7
Fagron	Prednicarbato	13c25-no6	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbato	13F11-N01	4
Fagron	Prednicarbato	13F11-No1	1
Fagron	Prednicarbato	13F11-NO1	1
Fagron	Prednicarbato	13G05-N03	5
Fagron	Prednicarbato	13I23-N04	8
Fagron	Prednicarbato	13l23-N04	1
Fagron	Prednicarbato	14A27-B02	2
Fagron	Prednicarbato	14a27-b02-291256	2
Fagron	Prednicarbato	14A27-B02-291256	17
Fagron	Prednicarbato	14A27-B02-291258	2
Fagron	Prednicarbato	14A27-B02-295793	1
Fagron	Prednicarbato	14A27-B02-295796	6
Fagron	Prednicarbato	14A27-B02-295797	7
Fagron	Prednicarbato	14B13-B31-291255	1
Fagron	Prednicarbato	14J16B06	1
Fagron	Prednicarbato	14J16-B06_303465	1
Fagron	Prednicarbato	14J16-B06-303465	14
Fagron	Prednicarbato	14J16B06303466	1
Fagron	Prednicarbato	15/22-B04-316799	1
Fagron	Prednicarbato	15D15-B03-30816	1
Fagron	Prednicarbato	15D15-B03308161	1
Fagron	Prednicarbato	15D15-B03-308161	9
Fagron	Prednicarbato	15D15-B03-308162	1
Fagron	Prednicarbato	15D15-B03-309682	1
Fagron	Prednicarbato	15E14-B03-355726	1
Fagron	Prednicarbato	15G10-B02	1
Fagron	Prednicarbato	15g10-b02-310848	1
Fagron	Prednicarbato	15G10-B02-310848	9
Fagron	Prednicarbato	15G10-B02-311819	1
Fagron	Prednicarbato	15G10-B02-314082	4
Fagron	Prednicarbato	15J22-B04	1
Fagron	Prednicarbato	15J22-B04-316799	6
Fagron	Prednicarbato	15J22-B04-318528	3
Fagron	Prednicarbato	15J22-B04-318930	6
Fagron	Prednicarbato	15J22-B04-321005	1
Fagron	Prednicarbato	15J22-BO4-316799	1
Fagron	Prednicarbato	15J-B04-316799	1
Fagron	Prednicarbato	16/27B01-332958	1
Fagron	Prednicarbato	16/27-B01-332958	2
Fagron	Prednicarbato	160314PC	1
Fagron	Prednicarbato	160518P	1
Fagron	Prednicarbato	16087410	1
Fagron	Prednicarbato	160902201	1
Fagron	Prednicarbato	1612-B01-325758	1
Fagron	Prednicarbato	16A18/B01	1
Fagron	Prednicarbato	16A18-B01-322732	6
Fagron	Prednicarbato	16E12-B01	2
Fagron	Prednicarbato	16E12-B01-325758	6
Fagron	Prednicarbato	16E12-B01-327344	3
Fagron	Prednicarbato	16E12-B01-32827	1
Fagron	Prednicarbato	16E12-B01-328270	6
Fagron	Prednicarbato	16E12-B01-330093	2
Fagron	Prednicarbato	16G09-B01-194722	2
Fagron	Prednicarbato	16J27-B01	2
Fagron	Prednicarbato	16j27b01330976	1
Fagron	Prednicarbato	16j27-b01-330976	1
Fagron	Prednicarbato	16J27-b01-330976	1
Fagron	Prednicarbato	16J27-B01-330976	12
Fagron	Prednicarbato	16J27-B01-330977	1
Fagron	Prednicarbato	16J27-B01-332958	13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbato	16J28-B01-330976	1
Fagron	Prednicarbato	17013804	1
Fagron	Prednicarbato	17104-805-343934	1
Fagron	Prednicarbato	17220407	2
Fagron	Prednicarbato	174J04-B05-343935	1
Fagron	Prednicarbato	17C27-B01	1
Fagron	Prednicarbato	17C27-B01-335530	10
Fagron	Prednicarbato	17C27-B01-335531	1
Fagron	Prednicarbato	17c27-b01-339079	1
Fagron	Prednicarbato	17C27-B01-339079	8
Fagron	Prednicarbato	17J04-B05	4
Fagron	Prednicarbato	17J04-B05-326113	1
Fagron	Prednicarbato	17J04-B05-340570	2
Fagron	Prednicarbato	17J04-B05-341872	9
Fagron	Prednicarbato	17j04-b05-343934	1
Fagron	Prednicarbato	17J04-B05-343934	9
Fagron	Prednicarbato	17J04-B05-343935	1
Fagron	Prednicarbato	17J04b05-346113	1
Fagron	Prednicarbato	17J04-B05-346113	10
Fagron	Prednicarbato	17Jo4B05343934	1
Fagron	Prednicarbato	1801013-01	4
Fagron	Prednicarbato	18194104	1
Fagron	Prednicarbato	18194105	1
Fagron	Prednicarbato	18194115	1
Fagron	Prednicarbato	18B17-B01-347486	1
Fagron	Prednicarbato	18B27-01-347486	1
Fagron	Prednicarbato	18B27-01-350264	1
Fagron	Prednicarbato	18B27-B01	2
Fagron	Prednicarbato	18B27-B01_347486	1
Fagron	Prednicarbato	18B27-B01-0001	1
Fagron	Prednicarbato	18B27-B01-346748	2
Fagron	Prednicarbato	18B27-B01-347486	20
Fagron	Prednicarbato	18B27-B01-350264	12
Fagron	Prednicarbato	18B27-B01-351177	3
Fagron	Prednicarbato	18E14-03-352631	1
Fagron	Prednicarbato	18E14-B03	5
Fagron	Prednicarbato	18E14B03-352560	1
Fagron	Prednicarbato	18E14-B03-352560	7
Fagron	Prednicarbato	18E14-B03-35260	1
Fagron	Prednicarbato	18E14-B03-352631	10
Fagron	Prednicarbato	18e14-b03-355726	1
Fagron	Prednicarbato	18E14-B03-355726	11
Fagron	Prednicarbato	18E-14-B03-355726	1
Fagron	Prednicarbato	18E14-B03-355727	3
Fagron	Prednicarbato	18J27-B01-332958	1
Fagron	Prednicarbato	194722	1
Fagron	Prednicarbato	19E14	1
Fagron	Prednicarbato	19E14-B01	1
Fagron	Prednicarbato	19E14-B01-191430	19
Fagron	Prednicarbato	19E14-B01-191431	3
Fagron	Prednicarbato	19G09-B01	3
Fagron	Prednicarbato	19G09-B01-194722	17
Fagron	Prednicarbato	19G09-B01-194724	3
Fagron	Prednicarbato	19J16-B04-197550	1
Fagron	Prednicarbato	19J16-B07	6
Fagron	Prednicarbato	19J16B07197550	1
Fagron	Prednicarbato	19J16-B07197550	1
Fagron	Prednicarbato	19J16-B07-197550	15
Fagron	Prednicarbato	19J16-B07-197552	3
Fagron	Prednicarbato	19J16-B07-197555	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbato	19J16-B07-20137002	1
Fagron	Prednicarbato	19J16-B07-201371	1
Fagron	Prednicarbato	19J16-B07-201372	15
Fagron	Prednicarbato	19J16-BO7-197550	1
Fagron	Prednicarbato	19J16-BO7-197552	1
Fagron	Prednicarbato	19J16-BO7-201372	1
Fagron	Prednicarbato	19J19-B07-197550	1
Fagron	Prednicarbato	20/18-B05-201649	1
Fagron	Prednicarbato	20003660007	1
Fagron	Prednicarbato	2001031-01	1
Fagron	Prednicarbato	20A21-B12	8
Fagron	Prednicarbato	20A21-B12-196767	1
Fagron	Prednicarbato	20A21-B12-1975501	2
Fagron	Prednicarbato	20A21-B12-197551	9
Fagron	Prednicarbato	20A21-B12-197553	3
Fagron	Prednicarbato	20A21-B12-197556	1
Fagron	Prednicarbato	20G23-B06	1
Fagron	Prednicarbato	20G23-B06-200074	1
Fagron	Prednicarbato	20g23-b06-200202	1
Fagron	Prednicarbato	20G23-B06-200202	2
Fagron	Prednicarbato	20I18-B05	3
Fagron	Prednicarbato	20I18-B05-2016409	1
Fagron	Prednicarbato	20I18-B05-201649	10
Fagron	Prednicarbato	20I8-B05-201649	1
Fagron	Prednicarbato	21a11-801-203584	1
Fagron	Prednicarbato	21A11-B01	6
Fagron	Prednicarbato	21A11-B01-201650	11
Fagron	Prednicarbato	21A11-B01-201651	1
Fagron	Prednicarbato	21A11-B01-2035804	2
Fagron	Prednicarbato	21A11B01203584	1
Fagron	Prednicarbato	21A11-B01-203584	31
Fagron	Prednicarbato	21A11-BO1-203584	1
Fagron	Prednicarbato	21F07-B17	1
Fagron	Prednicarbato	21F07-B17-216553	43
Fagron	Prednicarbato	21-F07-B17-216553	1
Fagron	Prednicarbato	21F07-B17-216554	3
Fagron	Prednicarbato	21FO7-0001	1
Fagron	Prednicarbato	21FO7-B17-216553	1
Fagron	Prednicarbato	21K24-B03-213700	2
Fagron	Prednicarbato	21K24-Bo3-213700	1
Fagron	Prednicarbato	22F03-B02-223102	2
Fagron	Prednicarbato	22F03-B02-227918	2
Fagron	Prednicarbato	22F03-B02-227919	1
Fagron	Prednicarbato	2762	1
Fagron	Prednicarbato	29091807	1
Fagron	Prednicarbato	2OG23-BO6-200074	1
Fagron	Prednicarbato	3251	1
Fagron	Prednicarbato	4111706	1
Fagron	Prednicarbato	701867	1
Fagron	Prednicarbato	701867-0001	2
Fagron	Prednicarbato	7061303	1
Fagron	Prednicarbato	8081403	1
Fagron	Prednicarbato	9E04-N02	1
Fagron	Prednicarbato	9G14-N06	1
Fagron	Prednicarbato	B01-2016500	1
Fagron	Prednicarbato	b01-2035804	1
Fagron	Prednicarbato	B01-2035804	9
Fagron	Prednicarbato	B01-203584	1
Fagron	Prednicarbato	B03-3557206	1
Fagron	Prednicarbato	B05-2016409	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbato	B06-2002002	1
Fagron	Prednicarbato	B07-2013702	1
Fagron	Prednicarbato	B12-1975501	5
Fagron	Prednicarbato	BO1-2035804	1
Fagron	Prednicarbato	htzthh	1
Fagron	Prednicarbato	na1668m	1
Fagron	Prednicarbato	NA2374M	2
Fagron	Prednicarbato	NT0555M13I23-N04	1
Fagron	Prednicarbato	NT0780M	2
Fagron	Prednicarbato	NU0823M	1
Fagron	Prednicarbato	NUO823M	1
Fagron	Prednicarbato	NV2209M	1
Fagron	Prednicarbato	NW0396M	1
Fagron	Prednicarbato	NX1422M	3
Fagron	Prednicarbato	NX1925M	3
Fagron	Prednicarbato	NX2297M	6
Fagron	Prednicarbato	NZ1045M	5
Fagron	Prednicarbato	PNC102/1020	6
Fargon / AHD	Prednicarbato	21A11-BO1-203584	1
Fargon/Phoenix 05.06.18	Prednicarbato	17J04-B05-343934	1
Fargon/Phönix	Prednicarbato	19J16-B07	1
Fargon	Prednicarbato	15J22-B04-318930	1
Fargon	Prednicarbato	16E12-B01_325758	1
Fargon	Prednicarbato	19G09-B01	1
Fargon	Prednicarbato	21A11-B01-203584	2
Farmabios S.p.A.	Prednicarbato	20003660009	1
Farmabios S.p.A/AHD	Prednicarbato	20000609006	1
Fiebig Palapharm	Prednicarbato	20000609004	1
Fiebig	Prednicarbato	17013804	1
Fiebig	Prednicarbato	17220408	1
Fiebig	Prednicarbato	18194105	1
Fiebig	Prednicarbato	20003660009	1
Fischar/ Noweda	Prednicarbato	21F07-B17-216553	1
Fragon/Sanacorp	Prednicarbato	NZ1845M	1
Fragron	Prednicarbato	NV0485M	1
Gehe amax	Prednicarbato	1507011-01	1
Gehe amax	Prednicarbato	15G10-B02-314082	1
Gehe amax	Prednicarbato	15J22-B04-316799	1
Gehe amax	Prednicarbato	1607012-01	1
Gehe amax	Prednicarbato	16J27-B01-330976	1
Gehe amax	Prednicarbato	1707022-01	2
Gehe amax	Prednicarbato	18B27-B01-350264	1
Gehe amax	Prednicarbato	20003660005	1
Gehe Rostock	Prednicarbato	19J16-B07-197550	1
Gehe Rostock	Prednicarbato	19J16-B07-201372	1
Gehe	Prednicarbato	12B14-N02	1
Gehe	Prednicarbato	13G05-n03	1
Gehe	Prednicarbato	13123-N04	1
Gehe	Prednicarbato	15446302	1
Gehe	Prednicarbato	15J22-B04-318930	1
Gehe	Prednicarbato	15J22-B04-321005	1
Gehe	Prednicarbato	1601058-01	1
Gehe	Prednicarbato	1605001-01	2
Gehe	Prednicarbato	1707022-01	3
GEHE	Prednicarbato	17315607	2
Gehe	Prednicarbato	1801013-01	5
Gehe	Prednicarbato	1805005-01	1
Gehe	Prednicarbato	1809015-01	4
GEHE	Prednicarbato	18194103	4
Gehe	Prednicarbato	18194105	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
GEHE	Prednicarbato	18194116	1
Gehe	Prednicarbato	18E14-B03	1
Gehe	Prednicarbato	1903023-01	3
Gehe	Prednicarbato	19032301	1
Gehe	Prednicarbato	19051601	1
Gehe	Prednicarbato	19122604	2
Gehe	Prednicarbato	19G09-B01	1
Gehe	Prednicarbato	19G09-B01-194722	2
Gehe	Prednicarbato	19J16-B07	1
Gehe	Prednicarbato	20003660004	1
Gehe	Prednicarbato	2009018-01	2
Gehe	Prednicarbato	20G23-B06	2
Gehe	Prednicarbato	21000991005	3
Gehe	Prednicarbato	21001161001	2
Gehe	Prednicarbato	21001161011	1
Gehe	Prednicarbato	21A11-B01	3
Gehe	Prednicarbato	21F07-B17	1
Gehe	Prednicarbato	21F07-B17-216553	1
Gehe	Prednicarbato	22000755002	2
Gehe	Prednicarbato	22000755007	1
Gehe	Prednicarbato	2204014-01	1
Gehe	Prednicarbato	22F03-B02-227918	1
Gehe	Prednicarbato	23001026001	5
Gehe	Prednicarbato	23001026002	2
Gehe	Prednicarbato	2304020-01	1
Gehe	Prednicarbato	2OG23-BO6-200202	1
GEHE	Prednicarbato	7529666	1
Gehe	Prednicarbato	B01-2016500	1
Gehe	Prednicarbato	C0333/1170101	1
Hedinger/ Sanacorp	Prednicarbato	15181403	1
Hedinger	Prednicarbato	16J27-B01-330976	2
Henry Lamotte	Prednicarbato	15D15-B03-308161	1
Hepart	Prednicarbato	17C27-B01-335530	1
JENNE	Prednicarbato	17220406	2
JENNE	Prednicarbato	17315603	1
Jenne	Prednicarbato	17J04-B05-346113	1
Jenne	Prednicarbato	18194105	1
Jenne	Prednicarbato	18194115	2
Jenne	Prednicarbato	1903023-01	1
Jenne	Prednicarbato	19J16-B07-197552	1
JENNE	Prednicarbato	22000755009	1
Jenne	Prednicarbato	23001026001	2
Jenne	Prednicarbato	P2019/91	1
Kehr Holdermann	Prednicarbato	23001026003	1
Kehr/Fargon	Prednicarbato	17J04-B05-346113	1
Kehr/Fargon	Prednicarbato	18B27-B01-350264	2
Kehr	Prednicarbato	16J27-B01-330976	1
Kehr	Prednicarbato	22000755006	1
Kehr	Prednicarbato	22000755010	3
Kehr	Prednicarbato	23001026001	4
Kehr	Prednicarbato	23001026002	1
Klenk	Prednicarbato	17014003	1
Krieger	Prednicarbato	2009018-01	1
Kriegeram 29.06.2018	Prednicarbato	17315605	1
Newchem / Gehe	Prednicarbato	18E14-B03-355726	1
Newchem / Gehe	Prednicarbato	19E14-B01-191430	1
Newchem / Gehe	Prednicarbato	B07-2013702	1
Newchem spa/Noweda	Prednicarbato	14A27-B02-291256	1
Newchem Spa/Sanacorp	Prednicarbato	16E12-B01	1
Newchem/ AHD	Prednicarbato	19122602	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Newchem/Phoenix	Prednicarbato	20I18-B05	1
NEWCHEM	Prednicarbato	19E14-B01-191430	2
Noveda	Prednicarbato	21A11-B01-203584	1
Noweda 17.11.17	Prednicarbato	17220407	1
Noweda Taucha	Prednicarbato	21001161010	1
Noweda	Prednicarbato	15446301	1
Noweda	Prednicarbato	161001	1
Noweda	Prednicarbato	17013804	2
Noweda	Prednicarbato	17315604	1
Noweda	Prednicarbato	17315605	1
Noweda	Prednicarbato	17315609	1
Noweda	Prednicarbato	17J04-B05-346113	1
Noweda	Prednicarbato	1801013-01	1
Noweda	Prednicarbato	1805005-01	1
Noweda	Prednicarbato	19122608	1
Noweda	Prednicarbato	20000366007	1
Noweda	Prednicarbato	20003660007	1
Noweda	Prednicarbato	21001161001	1
Noweda	Prednicarbato	2103017-01	4
Noweda	Prednicarbato	211867001	1
Noweda	Prednicarbato	21a11b01203584no	1
Noweda	Prednicarbato	21F07b17	1
Noweda	Prednicarbato	21K24-B03-2136699	1
Noweda	Prednicarbato	21K24-B03-213699	2
Noweda	Prednicarbato	22000755001	1
Noweda	Prednicarbato	2200755007	1
Noweda	Prednicarbato	2204014-01	1
Noweda	Prednicarbato	22F03-B02-223102	1
Noweda	Prednicarbato	22F03-B02-227918	1
Noweda	Prednicarbato	22F03-B02-227919	1
Noweda	Prednicarbato	23001025003	2
Noweda	Prednicarbato	23001026001	4
noweda	Prednicarbato	231001026003	1
Nowerda	Prednicarbato	17J04-B05-343934	1
Nowerda	Prednicarbato	18B27-B01-347486	1
Nowerda	Prednicarbato	18E14-B03-352560	1
Ph Eur/Ph	Prednicarbato	2103017-01	3
Phoenix 7.02.2020	Prednicarbato	1903023-01	1
phoenix	Prednicarbato	1323N04	1
Phoenix	Prednicarbato	16J27-b01-332958	1
Phoenix	Prednicarbato	17315604	3
Phoenix	Prednicarbato	17315605	1
Phoenix	Prednicarbato	17C27-B01-335530	1
Phoenix	Prednicarbato	1903023-02	1
Phoenix	Prednicarbato	19122602	1
Phoenix	Prednicarbato	20000609009	2
Phoenix	Prednicarbato	20003660007	1
Phoenix	Prednicarbato	22000755010	1
Phoenix	Prednicarbato	23001025003	1
Phoenix	Prednicarbato	23001026002	3
Phoenix	Prednicarbato	3070	1
Phoenix	Prednicarbato	3089	1
Phoenix	Prednicarbato	3097	1
Phoenix	Prednicarbato	3106	1
Phoenix	Prednicarbato	3119	1
Phoenix	Prednicarbato	3208	1
Phoenix	Prednicarbato	3239	1
Phoenix	Prednicarbato	3363	1
Phoenix	Prednicarbato	3408	1
Phoenix	Prednicarbato	B05-2016409	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix Gotha	Prednicarbato	17220408	1
Phönix	Prednicarbato	15J22-B04-318528	1
Phönix	Prednicarbato	16J27-B01-330976	1
Phönix	Prednicarbato	1707022-01	1
Phönix	Prednicarbato	18194104	2
Phönix	Prednicarbato	1903023-01	1
PHÖNIX	Prednicarbato	1903023-01	1
Phönix	Prednicarbato	20003660007	2
Phönix	Prednicarbato	2001031-01	4
Phönix	Prednicarbato	2009018-01	1
Phönix	Prednicarbato	20D07-F01370645	1
PHÖNIX	Prednicarbato	21001161001	1
Phönix	Prednicarbato	210301701	1
Phönix	Prednicarbato	2103017-01	2
phönix	Prednicarbato	21F07-B17-216553	1
Phönix	Prednicarbato	2204014-01	1
phönix	Prednicarbato	22F03-B02-223102	1
Phönix	Prednicarbato	22F03-B02-223102	1
Phönix	Prednicarbato	23001025003	1
Phönix	Prednicarbato	23001026002	2
Phönix	Prednicarbato	23003318006	1
Phönix	Prednicarbato	3134	1
Phönix	Prednicarbato	3154	1
Phönix	Prednicarbato	3185	1
Sanacop	Prednicarbato		3
Sanacorp, 01.03.17, ...	Prednicarbato	1687410	1
Sanacorp	Prednicarbato	11L23-N07	1
Sanacorp	Prednicarbato	17013804	1
Sanacorp	Prednicarbato	1707022-01	1
Sanacorp	Prednicarbato	17315604	2
Sanacorp	Prednicarbato	17315605	1
Sanacorp	Prednicarbato	18194105	1
Sanacorp	Prednicarbato	18194115	1
sanacorp	Prednicarbato	1903023-01	1
Sanacorp	Prednicarbato	20000609009	1
Sanacorp	Prednicarbato	20A-21-B12-197551	1
Sanacorp	Prednicarbato	20A21-B12-197553	1
Sanacorp	Prednicarbato	22000755009	2
Sanacorp	Prednicarbato	22F03-B02-223103	1
Sanacorp	Prednicarbato	23001026001	1
Sanacorp	Prednicarbato	B05-2016409	1
Sino Phyto	Prednicarbato	13224401	1
Sonnenberg-Apotheke	Prednicarbato	1607012-01	1
Symbiotica	Prednicarbato	2103017-01	1
Symbiotika	Prednicarbato	2009018-01	1

- 232 088 spectra from 1515 *Apo-Ident* customers from a total of 48 748 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednicarbato* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednicarbato* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	964	0	151 998
Type B	0	1297	0	200 787
Type C	0	3967	12	232 088

The substance/substance group *Prednicarbato* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3776 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5374 %)
Type C	100.0000 % (> 99.9007 %)	99.6984 % (> 99.6230 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20700	21572	30,21	205,06
20832	20832	0,00	187,59
20833	20832	2,37	186,73
21368	21368	0,00	155,13
21369	21368	2,82	155,56
21572	21572	0,00	202,31
21610	21610	0,00	165,51
21858	21858	0,00	194,33
22366	22366	0,00	147,83
25119	25119	0,00	213,53
25401	25401	0,00	211,09
25609	25609	0,00	211,19
26084	26084	0,00	206,15
26393	26084	23,79	202,59
27277	27277	0,00	212,13

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical

variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20773-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolona; Prednisolonum

Special notes

When selecting the *Prednisolona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisolona	14	11	453

Second-stage model

For differentiation of the substance/substance group *Prednisolona* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	44,36	–
Sulfato de polimixina B	107,64	–
⋮	⋮	⋮
Metilprednisolona	>50	45,50
Triancinolona acetonido	>50	67,78
Fluocinolona acetonida	>50	86,57
Betametasona	>50	95,18
Dexametasona	>50	96,60
Tirotricina	>50	130,84
Gramicidina	>50	157,31

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolona	12324202	20773	40	20121113
Caelo	Prednisolona	12324226	21303	39	1411271
Caelo	Prednisolona	13343105	21449	60	1411232
Caelo	Prednisolona	154000	22435	60	20160225*
Caelo	Prednisolona	154000	22435SI	59	20160225*
Caelo	Prednisolona	161343	22467	60	20160601*
Caelo	Prednisolona	161343	22467SI	44	20160601*
Caelo	Prednisolona	15400002	22783	40	20160225
Caelo	Prednisolona	15400002	22783SI	40	20160225
Caelo	Prednisolona	20001355	25192	40	20200528*
Caelo	Prednisolona	20001355	25192SI	40	20200528*
Euro OTC	Prednisolona	1212021-02	21604	60	1411270

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prednisolona	1212021-02	21604SI	48	1411270
Euro OTC	Prednisolona	1501047-01	21849	60	AR-15-FG-015509-01
Euro OTC	Prednisolona	1501047-01	21849SI	30	AR-15-FG-015509-01
Euro OTC	Prednisolona	1607011	22709	40	20160818*
Euro OTC	Prednisolona	1607011	22709SI	40	20160818*
Euro OTC	Prednisolona	2104012	25688	50	20210504*
Euro OTC	Prednisolona	2104012	25688SI	50	20210504*
Fagron	Prednisolona	13H07-B02-285592	21660	60	20130909
Fagron	Prednisolona	13H07-B02-285592	21660SI	60	20130909
Fagron	Prednisolona	14I10-B03-302263	22651	40	20141020
Fagron	Prednisolona	14I10-B03-302263	22651SI	40	20141020
Fagron	Prednisolona	16C15-B01-320761	22803	40	20160407
Fagron	Prednisolona	16C15-B01-320761	22803SI	36	20160407

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1176 spectra of 25 reference samples from the substance/substance group *Prednisolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.
- 151 786 spectra from a total of 2828 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 852 spectra of 23 reference samples from the substance/substance group *Prednisolona*.
- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisolona	172777	23846	40
Caelo	Prednisolona	21003654002	26414	40
Euro OTC	Prednisolona	1702020	23180	40
Euro OTC	Prednisolona	1905005	24602	40
Euro OTC	Prednisolona	2003019	25243	40
Euro OTC	Prednisolona	2205002	26208	40
Euro OTC	Prednisolona	2401004	27090	40
Fagron	Prednisolona	1108055-04	20855	40
Fagron	Prednisolona	16E09-B07-328220	23260	40
Fagron	Prednisolona	22B07-B20-220068	26289	30
Fagron	Prednisolona	24C07-B05-238310	27264	40
Caelo	Prednisolona	13343105	21451SI	60
Caelo	Prednisolona	161343	22467SI†	3
Caelo	Prednisolona	172777	23846SI	38
Caelo	Prednisolona	21003654002	26414SI	40
Euro OTC	Prednisolona	1702020	23180SI	21
Euro OTC	Prednisolona	1905005	24602SI	40
Euro OTC	Prednisolona	2003019	25243SI	40
Euro OTC	Prednisolona	2205002	26208SI	40
Euro OTC	Prednisolona	2401004	27090SI	40
Fagron	Prednisolona	16E09-B07-328220	23260SI	20
Fagron	Prednisolona	22B07-B20-220068	26289SI	40
Fagron	Prednisolona	24C07-B05-238310	27264SI	40

- 201 232 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2806 spectra from 941 *Apo-Ident* customers from 479 batches from the substance/substance group *Prednisolona*.

- Among them are spectra of independent samples from 453 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednisolona	1702020-02	1
	Prednisolona	21003654007	2
	Prednisolona	21003654010	1
	Prednisolona	21003654014	1
	Prednisolona	21003654016	2
	Prednisolona	21003654017	2
	Prednisolona	21003654021	5
	Prednisolona	2104012-01	2
	Prednisolona	21K27B04216441	1
	Prednisolona	2205002-01	14
	Prednisolona	22B07-B20-220050	2
	Prednisolona	22B07-B20-220068	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Prednisolona	22B07-B21	1
	Prednisolona	22B07-B21-222188	3
	Prednisolona	22B07-B21-222189	2
	Prednisolona	22B07-B21-224306	1
	Prednisolona	23002419002	2
	Prednisolona	23002419003	5
	Prednisolona	23002419006	3
	Prednisolona	23D24-B06-227228	3
	Prednisolona	23D24-B06-233604	2
	Prednisolona	2401004-01	1
	Prednisolona	B04-2336002	3
A.H. 05.03.13 ek: 14,08EUR	Prednisolona	12D30-N04	1
Aep	Prednisolona	21003654017	1
AHD/EuRho	Prednisolona	1905005-01	1
AHD	Prednisolona	121202103	1
AHD	Prednisolona	1212021-03	1
AHD	Prednisolona	160711-01	1
AHD	Prednisolona	16134308	1
AHD	Prednisolona	16134316	1
AHD	Prednisolona	1702020-01	1
AHD	Prednisolona	17277706	1
AHD	Prednisolona	21K27-B04-216441	2
AHD	Prednisolona	22B07-B21-222189	1
AHD	Prednisolona	23002419003	1
AHD	Prednisolona	24C07-B05-238309	1
Alliance Healtcare	Prednisolona	21003654002	1
Alliance Healthcare	Prednisolona	172777004	1
Alliance Healthcare	Prednisolona	17277723	1
Alliance Healthcare	Prednisolona	20001355002	1
Alliance Healthcare	Prednisolona	20004564006	2
Alliance Healthcare	Prednisolona	21003654012	1
Alliance Healthcare	Prednisolona	2205002-01	2
anzag	Prednisolona	14B18-B05-294966	1
Anzag	Prednisolona	20004564003	1
apo-Ident/ Sanacorp	Prednisolona	K04120190707	1
apomix	Prednisolona	16H04-B03-332930	1
Apotheke Mildenau	Prednisolona	1108055-04	3
Beiersdorf	Prednisolona	20004564003	1
Berkel AHK	Prednisolona	13343115	1
Bomastus / Alliance ...	Prednisolona	16134305	1
Bombastus	Prednisolona	1501047-02	1
Bombastus	Prednisolona	17F07-B05-341574	2
Bombastus	Prednisolona	17F07-B05-341578	2
Caelo	Prednisolona		2
Caelo	Prednisolona	10196604	1
Caelo	Prednisolona	10196606	1
Caelo	Prednisolona	10196611	3
Caelo	Prednisolona	10196622	2
Caelo	Prednisolona	10196625	1
Caelo	Prednisolona	10196626	6
Caelo	Prednisolona	10196627	7
Caelo	Prednisolona	11/26-N04	1
Caelo	Prednisolona	1212021-01	1
Caelo	Prednisolona	121202102	1
Caelo	Prednisolona	1212021-03	6
Caelo	Prednisolona	12171301	6
Caelo	Prednisolona	12171302	1
Caelo	Prednisolona	12171303	2
Caelo	Prednisolona	12171306	2
Caelo	Prednisolona	12185702	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolona	1232417	1
Caelo	Prednisolona	12324202	11
Caelo	Prednisolona	12324203	3
Caelo	Prednisolona	12324204	4
Caelo	Prednisolona	12324205	13
Caelo	Prednisolona	12324207	4
Caelo	Prednisolona	12324213	7
Caelo	Prednisolona	12324216	9
Caelo	Prednisolona	12324217	5
Caelo	Prednisolona	12324219	7
Caelo	Prednisolona	12324220	2
Caelo	Prednisolona	12324221	2
Caelo	Prednisolona	12324226	7
Caelo	Prednisolona	1234205	1
Caelo	Prednisolona	1234556	1
Caelo	Prednisolona	1250216	1
Caelo	Prednisolona	133414	1
Caelo	Prednisolona	13343101	1
Caelo	Prednisolona	13343104	11
Caelo	Prednisolona	13343105	4
Caelo	Prednisolona	13343106	8
Caelo	Prednisolona	13343107	1
Caelo	Prednisolona	13343111	4
Caelo	Prednisolona	13343112	4
Caelo	Prednisolona	13343113	1
Caelo	Prednisolona	13343114	5
Caelo	Prednisolona	13343115	9
Caelo	Prednisolona	13343116	4
Caelo	Prednisolona	13A07-N14	1
Caelo	Prednisolona	13E15-N06	4
Caelo	Prednisolona	14/10B03302265	1
Caelo	Prednisolona	14/10-B03-302266	1
Caelo	Prednisolona	1410B03302265	1
Caelo	Prednisolona	14A30-B02-294968	1
Caelo	Prednisolona	14B18-B05-294966	2
Caelo	Prednisolona	14G30-B14-302262	2
Caelo	Prednisolona	150104701	2
Caelo	Prednisolona	1501047-01	3
Caelo	Prednisolona	1501047-02	3
Caelo	Prednisolona	15055101	7
Caelo	Prednisolona	15055102	6
Caelo	Prednisolona	15055105	1
Caelo	Prednisolona	1511011	1
Caelo	Prednisolona	152006105	1
Caelo	Prednisolona	15206101	9
Caelo	Prednisolona	15206102	19
Caelo	Prednisolona	15206103	12
Caelo	Prednisolona	15206105	8
Caelo	Prednisolona	15206106	1
Caelo	Prednisolona	15206108	14
Caelo	Prednisolona	15400001	5
Caelo	Prednisolona	15400002	21
Caelo	Prednisolona	15400003	28
Caelo	Prednisolona	15400004	26
Caelo	Prednisolona	15400010	8
Caelo	Prednisolona	1540003	1
Caelo	Prednisolona	15K03-B04-314358	1
Caelo	Prednisolona	16034301	2
Caelo	Prednisolona	1607011-01	4
Caelo	Prednisolona	1613414	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolona	161343001	1
Caelo	Prednisolona	16134301	11
Caelo	Prednisolona	16134302	20
Caelo	Prednisolona	16134303	2
Caelo	Prednisolona	161343032	1
Caelo	Prednisolona	16134305	23
Caelo	Prednisolona	16134306	4
Caelo	Prednisolona	16134308	14
Caelo	Prednisolona	16134310	34
Caelo	Prednisolona	16134310-28122017/1	1
Caelo	Prednisolona	16134314	25
Caelo	Prednisolona	16134314/2120418	1
Caelo	Prednisolona	16134315	26
Caelo	Prednisolona	16134316	23
Caelo	Prednisolona	161343215	1
Caelo	Prednisolona	16A20-B03-316421	1
Caelo	Prednisolona	16C15-B01_320761	1
Caelo	Prednisolona	16C15-B01-320761	1
Caelo	Prednisolona	16C15-B01-321979	2
Caelo	Prednisolona	16C15-B01-324942	1
Caelo	Prednisolona	16C15-B02-324943	1
Caelo	Prednisolona	16E09-B07-328150	3
Caelo	Prednisolona	16E09-B07-328220	1
Caelo	Prednisolona	17020-01	1
Caelo	Prednisolona	1702020-01	3
Caelo	Prednisolona	1702020-02	3
Caelo	Prednisolona	1702020-03	3
Caelo	Prednisolona	172277710	1
Caelo	Prednisolona	17277004	1
Caelo	Prednisolona	1727702	2
Caelo	Prednisolona	1727704	2
Caelo	Prednisolona	1727710	1
Caelo	Prednisolona	1727716	2
Caelo	Prednisolona	1727718	1
Caelo	Prednisolona	1727720	1
Caelo	Prednisolona	1727723	1
Caelo	Prednisolona	1727770	1
Caelo	Prednisolona	172777002	35
Caelo	Prednisolona	17277702	13
Caelo	Prednisolona	17277703	15
Caelo	Prednisolona	17277704	42
Caelo	Prednisolona	17277706	18
Caelo	Prednisolona	17277710	14
Caelo	Prednisolona	17277711	24
Caelo	Prednisolona	17277714	1
Caelo	Prednisolona	17277716	42
Caelo	Prednisolona	17277718	3
Caelo	Prednisolona	17277719	1
Caelo	Prednisolona	17277720	33
Caelo	Prednisolona	17277723	16
Caelo	Prednisolona	1727777723	1
Caelo	Prednisolona	177277703	1
Caelo	Prednisolona	17f07-b05	1
Caelo	Prednisolona	17F07B05341574	1
Caelo	Prednisolona	17F07-B05-341574	2
Caelo	Prednisolona	17F07-B05-341578	1
Caelo	Prednisolona	18138113	1
Caelo	Prednisolona	18A29-B02-348041	1
Caelo	Prednisolona	18A29-B02-348540	2
Caelo	Prednisolona	18H07-B04-354523	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolona	18H07-B04-355631	2
Caelo	Prednisolona	1905005-01	2
Caelo	Prednisolona	1905005-02	1
Caelo	Prednisolona	19081504	1
Caelo	Prednisolona	20001355001	4
Caelo	Prednisolona	20001355002	13
Caelo	Prednisolona	20001355003	16
Caelo	Prednisolona	200013555002	1
Caelo	Prednisolona	20004564001	1
Caelo	Prednisolona	20004564002	6
Caelo	Prednisolona	20004564003	30
Caelo	Prednisolona	20004564005	24
Caelo	Prednisolona	20004564006	9
Caelo	Prednisolona	20004564008	7
Caelo	Prednisolona	20004564009	17
Caelo	Prednisolona	20021303	1
Caelo	Prednisolona	2004564002	1
Caelo	Prednisolona	20H20-B01-200829	1
Caelo	Prednisolona	21003645002	1
Caelo	Prednisolona	21003654002	21
Caelo	Prednisolona	21003654004	12
Caelo	Prednisolona	21003654006	1
Caelo	Prednisolona	21003654007	3
Caelo	Prednisolona	21003654010	7
Caelo	Prednisolona	21003654012	4
Caelo	Prednisolona	21003654014	2
Caelo	Prednisolona	21003654016	1
Caelo	Prednisolona	21003654017	2
Caelo	Prednisolona	21E04-B02-215330	1
Caelo	Prednisolona	21EO4-BO2-215330	1
Caelo	Prednisolona	21K27-B04-216439	3
Caelo	Prednisolona	22BO7-B20-220068	1
Caelo	Prednisolona	2413Q02105	1
Caelo	Prednisolona	3344	1
Caelo	Prednisolona	411092-1-P	1
Caelo	Prednisolona	4513U2105	1
Caelo	Prednisolona	4712I-02105	1
Caelo	Prednisolona	60367086	2
Caelo	Prednisolona	702020-01	1
Caelo	Prednisolona	9193501	1
Caelo	Prednisolona	AP201025-04	1
Caelo	Prednisolona	I-180716-15400003	1
Caelo	Prednisolona	I220216/2	1
Caelo	Prednisolona	k04c20121219	1
Caelo	Prednisolona	NEPL160202	1
Caelo	Prednisolona	NEPL180603	1
Caesar & Lorenz GmbH	Prednisolona	172777002	1
Caesar & Lorenz	Prednisolona	21003654012	1
Caesar & Loretz GmbH…	Prednisolona	172777002	1
Caesar & Loretz GmbH…	Prednisolona	17277720	1
Caesar & Loretz GmbH…	Prednisolona	20001355003	1
Caesar & Loretz GmbH…	Prednisolona	17277720	1
Caesar & Loretz GmbH…	Prednisolona	17277720	1
Caesar & Loretz GmbH…	Prednisolona	21003654010	1
Caesar & Loretz GmbH…	Prednisolona	17277718	2
Caesar & Loretz GmbH, Now	Prednisolona	21003654012	1
Caesar & Loretz GmbH…	Prednisolona	17277720	1
Caesar & Loretz GmbH/GEHE	Prednisolona	172777002	1
Caesar & Loretz GmbH/Gehe	Prednisolona	17277710	3
Caesar & Loretz GmbH/Gehe	Prednisolona	21003654017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Prednisolona	17277711	1
Caesar & Loretz GmbH...	Prednisolona	20004564005	1
Caesar & Loretz GmbH/Kehr	Prednisolona	17277710	1
Caesar & Loretz GmbH...	Prednisolona	17277711	1
Caesar & Loretz GmbH...	Prednisolona	20001355002	1
Caesar & Loretz GmbH...	Prednisolona	21003654002	1
Caesar & Loretz GmbH...	Prednisolona	20004564005	1
Caesar & Loretz GmbH...	Prednisolona	17277720	1
Caesar & Loretz GmbH...	Prednisolona	20001355003	1
Caesar & Loretz GmbH...	Prednisolona	20004564009	1
Caesar & Loretz GmbH...	Prednisolona	B09-1977207	1
Caesar & Loretz GmbH...	Prednisolona	17277723	1
Caesar & Loretz GmbH...	Prednisolona	1905005-01	1
Caesar & Loretz GmbH...	Prednisolona	20001355002	1
Caesar & Loretz GmbH...	Prednisolona	20004564003	1
Caesar & Loretz GmbH...	Prednisolona	20001355002	1
Caesar & Loretz GmbH	Prednisolona	12324205	1
Caesar & Loretz GmbH	Prednisolona	12324219	1
Caesar & Loretz GmbH	Prednisolona	15206101	2
Caesar & Loretz GmbH	Prednisolona	172777002	14
Caesar & Loretz GmbH	Prednisolona	172777004	1
Caesar & Loretz GmbH	Prednisolona	17277702	2
Caesar & Loretz GmbH	Prednisolona	17277704	4
Caesar & Loretz GmbH	Prednisolona	17277706	2
Caesar & Loretz GmbH	Prednisolona	17277710	1
Caesar & Loretz GmbH	Prednisolona	17277711	8
Caesar & Loretz GmbH	Prednisolona	17277716	11
Caesar & Loretz GmbH	Prednisolona	17277718	2
Caesar & Loretz GmbH	Prednisolona	17277720	12
Caesar & Loretz GmbH	Prednisolona	17277723	9
Caesar & Loretz GmbH	Prednisolona	190500502	1
Caesar & Loretz GmbH	Prednisolona	20001355002	5
Caesar & Loretz GmbH	Prednisolona	20001355003	6
Caesar & Loretz GmbH	Prednisolona	20004564002	7
Caesar & Loretz GmbH	Prednisolona	20004564003	10
Caesar & Loretz GmbH	Prednisolona	20004564005	11
Caesar & Loretz GmbH	Prednisolona	20004564006	7
Caesar & Loretz GmbH	Prednisolona	20004564008	5
Caesar & Loretz GmbH	Prednisolona	20004564009	10
Caesar & Loretz GmbH	Prednisolona	21003654002	7
Caesar & Loretz GmbH	Prednisolona	21003654004	6
Caesar & Loretz GmbH	Prednisolona	21003654007	2
Caesar & Loretz GmbH	Prednisolona	21003654010	4
Caesar & Loretz GmbH	Prednisolona	21003654012	1
Caesar & Loretz GmbH	Prednisolona	21003654014	2
Caesar & Loretz GmbH	Prednisolona	21003654021	1
Caesar & Loretz Hild...	Prednisolona	17277723	1
Caesar & Loretz Hilden	Prednisolona	17277711	1
Caesar & Loretz Hilden	Prednisolona	17277716	1
Caesar & Loretz Hilden	Prednisolona	20001355003	1
Caesar & Loretz	Prednisolona	20001355002	2
Caesar u. Loretz/Noweda	Prednisolona	16134301	1
Caesar&Loretz GmbH/Anzag	Prednisolona	13343112	1
Caesar/Lorenz	Prednisolona	12324204	1
Caesar+ Loretz GmbH	Prednisolona	20004564003	1
Caleo/Jenne 28.04.22...	Prednisolona	20004564006	1
Caolo- Noweda	Prednisolona	15206103	1
Cealo/Noweda	Prednisolona	1526108	1
Cealo	Prednisolona	16134305	2
Cealo	Prednisolona	17277703	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo	Prednisolona	2001355002	1
Cealo	Prednisolona	21003654002	1
Celo/Noweda	Prednisolona	1727703	1
CVH/Jenne	Prednisolona	19K27-B09	1
Ebert & Jacobi	Prednisolona	1212021-03	2
EU.RHO.Pharm	Prednisolona	K04120190707	1
EuRho/AHD	Prednisolona	1702020-03	1
EuRho/Jenne	Prednisolona	1108055-04	2
EuRho/Noweda	Prednisolona	1702020-01	1
EuRho	Prednisolona	1012012-01	1
EuRho	Prednisolona	1012012-02	2
EuRho	Prednisolona	1108055-03	2
EuRho	Prednisolona	1212021-02	1
EuRho	Prednisolona	1702020-01	1
EuRho	Prednisolona	1702020-02	1
EuRho	Prednisolona	190500501	1
EuRho	Prednisolona	2003019-01	1
Euro Gehe	Prednisolona	1702020-03	1
Euro OCT/Noweda	Prednisolona	1501047-02	1
Euro OTC	Prednisolona		1
Euro OTC	Prednisolona	1012012-02	2
Euro OTC	Prednisolona	1108055-01	1
Euro OTC	Prednisolona	1108055-02	2
Euro OTC	Prednisolona	1108055-03	10
Euro OTC	Prednisolona	110805504	4
Euro OTC	Prednisolona	1108055-04	17
Euro OTC	Prednisolona	118055-04	1
Euro OTC	Prednisolona	12021-03	1
Euro OTC	Prednisolona	121021-01	2
Euro OTC	Prednisolona	1212021	1
Euro OTC	Prednisolona	121202101	1
Euro OTC	Prednisolona	1212021-01	30
Euro OTC	Prednisolona	121202102	2
Euro OTC	Prednisolona	1212021-02	27
Euro OTC	Prednisolona	1212021-03	40
Euro OTC	Prednisolona	121221-03	1
Euro OTC	Prednisolona	1314Q2105	1
Euro OTC	Prednisolona	13343104	1
Euro OTC	Prednisolona	14/10-B03-302263	1
Euro OTC	Prednisolona	1501047	1
Euro OTC	Prednisolona	150104701	3
Euro OTC	Prednisolona	1501047-01	27
Euro OTC	Prednisolona	1501047-02	18
Euro OTC	Prednisolona	1501047-03	6
Euro OTC	Prednisolona	150104743	1
Euro OTC	Prednisolona	150104747-01	1
Euro OTC	Prednisolona	15010477-01	1
Euro OTC	Prednisolona	1501074-02	1
Euro OTC	Prednisolona	15014047-02	1
Euro OTC	Prednisolona	15206108	1
Euro OTC	Prednisolona	15400010	1
Euro OTC	Prednisolona	15K03-B04-314226	1
Euro OTC	Prednisolona	1607011-01	42
Euro OTC	Prednisolona	16134308	3
Euro OTC	Prednisolona	16134316	2
Euro OTC	Prednisolona	16E09-B07-329686	2
Euro OTC	Prednisolona	170202001	2
Euro OTC	Prednisolona	1702020-01	55
Euro OTC	Prednisolona	170202002	3
Euro OTC	Prednisolona	1702020-02	52

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prednisolona	1702020-03	25
Euro OTC	Prednisolona	170202-03	3
Euro OTC	Prednisolona	1702020-30	1
Euro OTC	Prednisolona	170202201	1
Euro OTC	Prednisolona	172020-03	1
Euro OTC	Prednisolona	18A29-B02-348044	1
Euro OTC	Prednisolona	18H07-B04	1
Euro OTC	Prednisolona	190500-01	2
Euro OTC	Prednisolona	19050005-01	1
Euro OTC	Prednisolona	1905005	1
Euro OTC	Prednisolona	1905005_01	1
Euro OTC	Prednisolona	190500501	6
Euro OTC	Prednisolona	1905005-01	85
Euro OTC	Prednisolona	1905005-02	30
Euro OTC	Prednisolona	1905005-0P-191223-5	1
Euro OTC	Prednisolona	190500t-02	1
Euro OTC	Prednisolona	200301901	2
Euro OTC	Prednisolona	2003019-01	44
Euro OTC	Prednisolona	200560	1
Euro OTC	Prednisolona	210401201	1
Euro OTC	Prednisolona	2104012-01	20
Euro OTC	Prednisolona	30042014B	1
Euro OTC	Prednisolona	501047-01	1
Euro OTC	Prednisolona	NEPL110103	1
Euro/ Sanacorp	Prednisolona	121202103	1
Euro/Gehe	Prednisolona	1702020-01	1
Euro/Phoenix	Prednisolona	190500501	1
Euro/Phoenix	Prednisolona	190500502	1
Euro/Phönix	Prednisolona	1702020-01	1
Euro/Phönix	Prednisolona	1905005-01	1
euroct/gehe	Prednisolona	1212021-01	1
euroct/Gehe	Prednisolona	1212021-01	1
Europh/Ph	Prednisolona	1702020-02	1
Europharm/Otto	Prednisolona	1108055-03	1
Europharm/Otto	Prednisolona	1108055-04	5
europharma	Prednisolona	1002001240	1
Fagron	Prednisolona		1
Fagron	Prednisolona	10J04-N06	1
Fagron	Prednisolona	11D13-N05	2
Fagron	Prednisolona	11G22-N08	1
Fagron	Prednisolona	11J26-N04	2
Fagron	Prednisolona	1212021-02	2
Fagron	Prednisolona	12324216	1
Fagron	Prednisolona	12c22-N05	1
Fagron	Prednisolona	12C22-N05	7
Fagron	Prednisolona	12D30-N04	9
Fagron	Prednisolona	12D30-NO4	1
Fagron	Prednisolona	12K14-N03	10
Fagron	Prednisolona	12K14-NO3	1
Fagron	Prednisolona	130F-N04	1
Fagron	Prednisolona	13343106	1
Fagron	Prednisolona	13A07N14	1
Fagron	Prednisolona	13A07-N14	6
Fagron	Prednisolona	13DE15-N06	1
Fagron	Prednisolona	13E13-N06	1
Fagron	Prednisolona	13E15-N06	16
Fagron	Prednisolona	13E15-NO6	1
Fagron	Prednisolona	13G03-B09	1
Fagron	Prednisolona	13H07-B02	2
Fagron	Prednisolona	13H07-B020	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolona	13H07-B02-285590	3
Fagron	Prednisolona	13H07-B02-285592	4
Fagron	Prednisolona	13H07-B02-285593	4
Fagron	Prednisolona	13H07-B02-285593	1
Fagron	Prednisolona	13H7-B02-285590	1
Fagron	Prednisolona	13J28-B06	2
Fagron	Prednisolona	13J28-B06-289670	3
Fagron	Prednisolona	14/10-B03	1
Fagron	Prednisolona	14/10B03302265	1
Fagron	Prednisolona	14/10-B03-302265	4
Fagron	Prednisolona	14/10-B03-302266	2
Fagron	Prednisolona	14/10-B03-302269	1
Fagron	Prednisolona	14/10-B03-302271	1
Fagron	Prednisolona	1410-B03	1
Fagron	Prednisolona	1410-B03-302269	2
Fagron	Prednisolona	14818-B05-294966	1
Fagron	Prednisolona	14A30-B02-294968	5
Fagron	Prednisolona	14B18-B05	1
Fagron	Prednisolona	14B18-B05294966	1
Fagron	Prednisolona	14B18-B05-294966	10
Fagron	Prednisolona	14B18-B05-294969	2
Fagron	Prednisolona	14B18-Bo5-294966	1
Fagron	Prednisolona	14G30-B14	1
Fagron	Prednisolona	14G30-B14-302262	4
Fagron	Prednisolona	14I10-B03	1
Fagron	Prednisolona	14I10-B03-302265	2
Fagron	Prednisolona	14I10-B03-302266	1
Fagron	Prednisolona	14i10-b03-302269	1
Fagron	Prednisolona	14I10-B03-302269	3
Fagron	Prednisolona	14l10-B03302265	1
Fagron	Prednisolona	14L10-B03-302269	1
Fagron	Prednisolona	1501047-02	1
Fagron	Prednisolona	150528P	1
Fagron	Prednisolona	15B18-B05-294969	1
Fagron	Prednisolona	15D14-B01	1
Fagron	Prednisolona	15D14-B01-308425	3
Fagron	Prednisolona	15K03_B04_314226	1
Fagron	Prednisolona	15K03-B04	1
Fagron	Prednisolona	15k03-b04-314226	1
Fagron	Prednisolona	15K03B04314226	1
Fagron	Prednisolona	15K03-B04-314226	13
Fagron	Prednisolona	15K03-B04-314357	2
Fagron	Prednisolona	15K03-B04-314358	6
Fagron	Prednisolona	15K03-B04-314869	2
Fagron	Prednisolona	15KO3-B04-314226	1
Fagron	Prednisolona	1607011-01	2
Fagron	Prednisolona	16134310	1
Fagron	Prednisolona	16A20-B03	4
Fagron	Prednisolona	16A20-B03-316420	7
Fagron	Prednisolona	16A20-B03-316421	1
Fagron	Prednisolona	16A20-B03-319015	7
Fagron	Prednisolona	16c15-802	1
Fagron	Prednisolona	16C15-B01	1
Fagron	Prednisolona	16C15-B01-319992	2
Fagron	Prednisolona	16c15-B01-320761	2
Fagron	Prednisolona	16C15B01320761	2
Fagron	Prednisolona	16C15-B01-320761	4
Fagron	Prednisolona	16C15B01321979	1
Fagron	Prednisolona	16C15-B01-321979	15
Fagron	Prednisolona	16C15-B01-324942	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolona	16c15-b02	1
Fagron	Prednisolona	16C15-B02	1
Fagron	Prednisolona	16C15-B02-324943	6
Fagron	Prednisolona	16C15-B02-324945	1
Fagron	Prednisolona	16C15-B01-321979	1
Fagron	Prednisolona	16C19-B07-353242	1
Fagron	Prednisolona	16E09/B07/328220	1
Fagron	Prednisolona	16E09-B07_328220	1
Fagron	Prednisolona	16E09-B07-328150	17
Fagron	Prednisolona	16E09-B07-328220	7
Fagron	Prednisolona	16e09-B07-329686	1
Fagron	Prednisolona	16E09-B07-329686	1
Fagron	Prednisolona	16E09-B075411	1
Fagron	Prednisolona	16H04b03332929	1
Fagron	Prednisolona	16H04-B03-332929	15
Fagron	Prednisolona	16H04-B03-332930	8
Fagron	Prednisolona	16K27-B09-200489	1
Fagron	Prednisolona	17014-801-340448	1
Fagron	Prednisolona	17020201	1
Fagron	Prednisolona	1711021A	1
Fagron	Prednisolona	1717M-02105	1
Fagron	Prednisolona	17D14-B01	1
Fagron	Prednisolona	17D14b01338573	1
Fagron	Prednisolona	17D14-B01-338573	5
Fagron	Prednisolona	17D14-Bo1-338573	1
Fagron	Prednisolona	17F07-B05	3
Fagron	Prednisolona	17F07-B05_341574	1
Fagron	Prednisolona	17F07-B05-341574	6
Fagron	Prednisolona	17F07-B05-341575	5
Fagron	Prednisolona	17F07-B05-341578	2
Fagron	Prednisolona	17g2828-b03-345539	1
Fagron	Prednisolona	17G28-B03	3
Fagron	Prednisolona	17G28-B03-345538	10
Fagron	Prednisolona	17G28-B03-345539	4
Fagron	Prednisolona	17G2B03-345538	1
Fagron	Prednisolona	18A29-B02	2
Fagron	Prednisolona	18A29-B02-348041	2
Fagron	Prednisolona	18A29-B02-348044	1
Fagron	Prednisolona	18A29-B02-348540	4
Fagron	Prednisolona	18C19-B07	2
Fagron	Prednisolona	18C19-B07-351225	5
Fagron	Prednisolona	18C19B07351226	1
Fagron	Prednisolona	18C19-B07-351226	4
Fagron	Prednisolona	18C19-B07-353242	5
Fagron	Prednisolona	18H07-804	1
Fagron	Prednisolona	18H07-B04	3
Fagron	Prednisolona	18H07-B04_355630	1
Fagron	Prednisolona	18h07-b04-353326	1
Fagron	Prednisolona	18H07-B04-353326	4
Fagron	Prednisolona	18H07-B04-354523	10
Fagron	Prednisolona	18H07-B04-355630	6
Fagron	Prednisolona	18H07B04355631	1
Fagron	Prednisolona	18H07-B04-355631	6
Fagron	Prednisolona	18H7-B04-355631	1
Fagron	Prednisolona	1905005-01	3
Fagron	Prednisolona	194548	1
Fagron	Prednisolona	19-B07-351226	1
Fagron	Prednisolona	19E28-814-191220	1
Fagron	Prednisolona	19e28-B13	1
Fagron	Prednisolona	19E28-B13	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolona	19E28B13191224	1
Fagron	Prednisolona	19E28-B13-191224	9
Fagron	Prednisolona	19E28-B14	3
Fagron	Prednisolona	19E28-B14-1911225	1
Fagron	Prednisolona	19E28-B14-191220	16
Fagron	Prednisolona	19E28-B14-1912220	1
Fagron	Prednisolona	19H19-302	1
Fagron	Prednisolona	19H19-B02	3
Fagron	Prednisolona	19H19-B02-194547	1
Fagron	Prednisolona	19H19-B02-194548	10
Fagron	Prednisolona	19H19-B02-194549	2
Fagron	Prednisolona	19H19-BO2-194548	2
Fagron	Prednisolona	19K27-809	1
Fagron	Prednisolona	19K27-B09	2
Fagron	Prednisolona	19K27-B09-1977207	1
Fagron	Prednisolona	19k27b09197727	1
Fagron	Prednisolona	19K27-B09-197727	14
Fagron	Prednisolona	19k27-b09-200489	1
Fagron	Prednisolona	19K27B09-200489	1
Fagron	Prednisolona	19K27-B09-200489	10
Fagron	Prednisolona	19K27B09200517	2
Fagron	Prednisolona	19K27-B09-200517	6
Fagron	Prednisolona	20004564003	1
Fagron	Prednisolona	200738	1
Fagron	Prednisolona	20H20-B01	2
Fagron	Prednisolona	20H20-B01_202715	1
Fagron	Prednisolona	20H20B01200714	1
Fagron	Prednisolona	20H20-B01-200736	1
Fagron	Prednisolona	20H20-B01-200738	7
Fagron	Prednisolona	20h20B01-200829	1
Fagron	Prednisolona	20H20-B01-200829	3
Fagron	Prednisolona	20H20-B01-202715	6
Fagron	Prednisolona	20H20-B01-204241	2
Fagron	Prednisolona	20H20-BO1-200829	1
Fagron	Prednisolona	21/07-B03-213752	1
Fagron	Prednisolona	21107-B03	1
Fagron	Prednisolona	211217(19519-B02-194548)	1
Fagron	Prednisolona	21E04-B02215330	2
Fagron	Prednisolona	21E04-B02-215330	10
Fagron	Prednisolona	21I07B03213148	1
Fagron	Prednisolona	21I07-B03-213148	1
Fagron	Prednisolona	21I07-B03-213752	5
Fagron	Prednisolona	21k27-b04-216439	1
Fagron	Prednisolona	21K27-B04-216439	5
Fagron	Prednisolona	21K27-BO4-216441	1
Fagron	Prednisolona	22807-820-220050	1
Fagron	Prednisolona	22B07-B20-220050	2
Fagron	Prednisolona	22b07-B21-222188	1
Fagron	Prednisolona	23E30-B04-234317	1
Fagron	Prednisolona	2834	1
Fagron	Prednisolona	2915E-02105	1
Fagron	Prednisolona	3518E-02105	1
Fagron	Prednisolona	4313E-02105	1
Fagron	Prednisolona	613Q-02105	1
Fagron	Prednisolona	8576886	1
Fagron	Prednisolona	B01-2007308	1
Fagron	Prednisolona	B01-2008209	2
Fagron	Prednisolona	B02-1945408	1
Fagron	Prednisolona	B02-2153300	1
Fagron	Prednisolona	B09-1977207	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolona	B09-1977208	1
Fagron	Prednisolona	B09-2004809	2
Fagron	Prednisolona	b14-1912200	1
Fagron	Prednisolona	BO9-1977207	1
Fagron	Prednisolona	K04C20121006	1
Fagron	Prednisolona	K04C20130203M	1
Fagron	Prednisolona	K04C20131102	1
Fagron	Prednisolona	K04C20140502	2
Fagron	Prednisolona	KO4C20121006	1
Fagron	Prednisolona	NEPL151202	1
Fagron	Prednisolona	NEPL160202	1
Fagron	Prednisolona	NEPL160705	1
Fagron	Prednisolona	NEPL170209	2
Fagron	Prednisolona	NEPL170210	1
Fagron	Prednisolona	NEPL170605	3
Fagron	Prednisolona	NEPL1711	1
Fagron	Prednisolona	NEPL171111	1
Fagron	Prednisolona	NEPL180603	1
Fagron	Prednisolona	NEPL190306	1
Fagron	Prednisolona	NEPL190405	4
Fagron	Prednisolona	nepl190811	1
Fagron	Prednisolona	NEPL190811	2
Fagron	Prednisolona	NEPL200714	1
Fagron	Prednisolona	NEPL211006	2
Fagron	Prednisolona	NPL190306	1
Fargo	Prednisolona	12D30-N04	1
Fargon / AHD	Prednisolona	18C19-B07-351226	1
Fargon/AHD	Prednisolona	18A29-B02-348044	1
Fargon/Kehr	Prednisolona	22B07-B21-224304	1
Fargon	Prednisolona	16134308	1
Fargon	Prednisolona	19E28-B14-191220	1
Fargon	Prednisolona	FPO1409P	1
Fargron	Prednisolona	13E15-N06	1
Fischar/Gehe	Prednisolona	14A30-B02-294968	1
Fragon/Phoenix	Prednisolona	15K03-B04-314226	1
Fragon/Phoenix	Prednisolona	16C15-B02-324943	1
Fragon	Prednisolona	18C19-B07-351225	1
Gehe amax	Prednisolona	1501047-01	3
Gehe amax	Prednisolona	1607011-01	2
Gehe amax	Prednisolona	16134310	1
Gehe amax	Prednisolona	1702020-01	1
Gehe amax	Prednisolona	1702020-02	1
Gehe amax	Prednisolona	17277704	1
Gehe amax	Prednisolona	17277720	2
Gehe amax	Prednisolona	1905005-01	2
Gehe/Fragon	Prednisolona	16E09B07328150	1
Gehe	Prednisolona	1212021-01	4
Gehe	Prednisolona	1212021-02	1
Gehe	Prednisolona	12324216	2
Gehe	Prednisolona	12C22-N05	1
Gehe	Prednisolona	13343107	1
Gehe	Prednisolona	13A07-N14	2
Gehe	Prednisolona	13E15-No6	1
Gehe	Prednisolona	14A30-B02-294968	1
Gehe	Prednisolona	1501047-01	4
Gehe	Prednisolona	16134302	1
Gehe	Prednisolona	16134314	1
Gehe	Prednisolona	16C15-B01	1
Gehe	Prednisolona	16C15-B01-321979	1
Gehe	Prednisolona	16C-15-B02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Prednisolona	16E09-B07	1
GEHE	Prednisolona	1702020-02	1
Gehe	Prednisolona	172777002	1
Gehe	Prednisolona	17277710	1
Gehe	Prednisolona	17277718	3
Gehe	Prednisolona	17F07-B05-341574	1
Gehe	Prednisolona	17G28-B03	1
Gehe	Prednisolona	18H07-B04	1
Gehe	Prednisolona	18H07-B04-355630	2
Gehe	Prednisolona	18H07-B04-355631	1
Gehe	Prednisolona	19E28-B14_191220	1
Gehe	Prednisolona	19H19-B02	1
Gehe	Prednisolona	20004564002	1
GEHE	Prednisolona	21K27-B04-216441	1
Gehe	Prednisolona	23E30-B04-235950	1
Gehe-Fragon	Prednisolona	14B18B05294966	1
GUMO	Prednisolona	19K27-B09_20048	1
Hedinger	Prednisolona	P2018/116	1
Henan / Ebert	Prednisolona	16134316	1
Henan Lihua/Gehe	Prednisolona	1501047-01	2
Henan/Noweda	Prednisolona	K04120190303	1
Ichthyol / Phoenix	Prednisolona	16C15-B01-320761	1
Ichthyol gesellschaft	Prednisolona	15400003	1
Jenne / Fargon	Prednisolona	14B18B05294966	2
Kehr	Prednisolona	23D24-B06-227228	1
Kehr	Prednisolona	23D24-B06-227230	1
Krieger	Prednisolona	3416	1
Leyh Pharma	Prednisolona	16A20-B03-319015	1
Nachprüfung	Prednisolona	2082019-8	1
Noweda	Prednisolona	10196626	2
Noweda	Prednisolona	1108055-05	1
Noweda	Prednisolona	1212021-02	1
Noweda	Prednisolona	15206101	1
Noweda	Prednisolona	1607011-01	1
Noweda	Prednisolona	16134316	1
Noweda	Prednisolona	16H04-B03-332930	1
Noweda	Prednisolona	18A29-B02-348041	1
Noweda	Prednisolona	1905005-01	1
Noweda	Prednisolona	19E28-B14-191220	2
Noweda	Prednisolona	20004564003	1
Noweda	Prednisolona	20004564005	1
Noweda	Prednisolona	20H20-B01-200829	1
Noweda	Prednisolona	21003654002	1
Noweda	Prednisolona	21107-B03-213752	1
Noweda	Prednisolona	2205002-01	5
Noweda-Euro	Prednisolona	K04I20210211	2
Otto Geilenkirchen	Prednisolona	16134305	1
Ph.Eur 8.0	Prednisolona	14/10-B03-302263	2
Phoenix 01.08.2017 8,69EUR	Prednisolona	16E09-B07-328150	1
Phoenix 14.11.2017	Prednisolona	16H04-B03-332929	1
phoenix 5.4.2013	Prednisolona	1108055-04	1
Phoenix	Prednisolona	11j26-N04	2
Phoenix	Prednisolona	15400003	1
Phoenix	Prednisolona	16134310	1
Phoenix	Prednisolona	16134315	1
Phoenix	Prednisolona	16H04B03332930	1
Phoenix	Prednisolona	17277703	1
Phoenix	Prednisolona	17277711	1
Phoenix	Prednisolona	20004564005	4
Phoenix	Prednisolona	20004564009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Prednisolona	200602406	1
Phoenix	Prednisolona	3220	1
Phönix Gotha	Prednisolona	1232417	1
Phönix Gotha	Prednisolona	12324213	1
Phönix Gotha	Prednisolona	12324217	1
Phönix Gotha	Prednisolona	13343105	1
Phönix Gotha	Prednisolona	13343111	1
Phönix Gotha	Prednisolona	13343112	2
Phönix/Euro	Prednisolona	1501047-03	1
Phönix/Euro	Prednisolona	1702020-02	1
Phönix/Fagon	Prednisolona	16C15-B01-324942	1
Phönix	Prednisolona	12324216	1
Phönix	Prednisolona	13A07N14	1
Phönix	Prednisolona	13E15-N06	2
Phönix	Prednisolona	14B18-B05-294966	1
Phönix	Prednisolona	16134305	1
Phönix	Prednisolona	16134314	1
Phönix	Prednisolona	17277704	1
phönix	Prednisolona	17277716	1
Phönix	Prednisolona	17277720	1
Phönix	Prednisolona	17277723	2
Phönix	Prednisolona	18A29B02348540	1
Phönix	Prednisolona	19K27-B09-200489	2
Phönix	Prednisolona	2003019-01	1
Röntgen	Prednisolona	170202001	1
Sanacorp WE:01.08.20…	Prednisolona	1501047-01	1
Sanacorp	Prednisolona	1108055-03	1
Sanacorp	Prednisolona	12324221	1
Sanacorp	Prednisolona	13343112	1
Sanacorp	Prednisolona	13E15-N06	1
Sanacorp	Prednisolona	13H07-B02-285592	1
Sanacorp	Prednisolona	13j28-b06-289670	1
sanacorp	Prednisolona	14/10-B03-302266	1
Sanacorp	Prednisolona	14/10-B03-302269	1
Sanacorp	Prednisolona	16134310	1
Sanacorp	Prednisolona	16H04-B03_332930	1
Sanacorp	Prednisolona	17F07-B05-341575	1
Sanacorp	Prednisolona	18AB02	1
Sanacorp	Prednisolona	20001355002	1
Sanacorp	Prednisolona	21I07-B03-213752	1
Sanacorp	Prednisolona	21K27-B04-0002	1
Sanacorp	Prednisolona	22B07-B20-220068	1
Sanacorp	Prednisolona	22B07-B21-224306	1
Sanacorp	Prednisolona	23002419002	1
Sanacorp	Prednisolona	23002419003	1
Sanacorp	Prednisolona	23E30-B04-235951	1
Sonnenberg-Apotheke	Prednisolona	12324219	1
Tianjin Tianyao Pharm/AHD	Prednisolona	19H19-B02-194548	1
Tianyao Pharma/Phönix	Prednisolona	1212021-01	1
Tianyao Pharma/Phönix	Prednisolona	NEPL110103	1

- 233 261 spectra from 1514 *Apo-Ident* customers from a total of 48 783 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1162	14	151 786
Type B	0	852	0	201 232
Type C	0	2760	46	233 261

The substance/substance group *Prednisolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	98.8095 % (> 98.5544 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2958 %)
Type C	100.0000 % (> 99.9007 %)	98.3607 % (> 98.2537 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20773	21303	9,32	155,59
21303	21303	0,00	150,76
21449	21449	0,00	150,64
21604	21604	0,00	150,61
21660	21449	3,77	152,86
21849	21849	0,00	139,69
22435	22435	0,00	151,70
22467	22467	0,00	140,93
22651	21449	9,54	157,97
22709	22709	0,00	147,35
22783	22435	3,62	151,94
22803	22435	9,80	149,67
25192	25192	0,00	147,15
25688	25688	0,00	151,87

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20002-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisona

Special notes

When selecting the *Prednisona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisona	6	8	58

Second-stage model

For differentiation of the substance/substance group *Prednisona* the following second-stage model is used:

- Submodelo 08

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	69,55	–
⋮	⋮	⋮
Acetato de prednisolona	>50	37,12
Cloridrato de efedrina	>50	137,13

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisona	12232716	21408	60	20120829
Caelo	Prednisona	12232716	21409	60	20120829
Caelo	Prednisona	192455	24895	40	31102019*
Euro OTC	Prednisona	1401042-02	21616	60	1605276
Euro OTC	Prednisona	1604051	22557	40	20160523*
Euro OTC	Prednisona	1604051	22557SI	40	20160523*
Fagron	Prednisona	13C14-B40-289148	21573	60	20131223
Fagron	Prednisona	16J19-B02-328642	23227	40	20161221

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 8 reference samples from the substance/substance group *Prednisona*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 562 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 769 spectra of 20 reference samples from the substance/substance group *Prednisona*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisona	171665	23341	20
Caelo	Prednisona	17166504	23578	30
Caelo	Prednisona	21003706	25993	40
Caelo	Prednisona	23000981	26974	40
Euro OTC	Prednisona	1702008	23179	40
Fagron	Prednisona	22A14-B08-213641	26133	40
Fagron	Prednisona	23A04-B03-226162	26618	40
Fagron	Prednisona	24A30-B09-237512	27373	40
Caelo	Prednisona	12232716	21408SI†	60
Caelo	Prednisona	12232716	21409SI†	60
Caelo	Prednisona	171665	23341SI	30
Caelo	Prednisona	17166504	23578SI	30
Caelo	Prednisona	192455	24895SI†	40
Caelo	Prednisona	21003706	25993SI	40
Caelo	Prednisona	23000981	26974SI	40
Euro OTC	Prednisona	1702008	23179SI	29
Fagron	Prednisona	16J19-B02-328642	23227SI†	30
Fagron	Prednisona	22A14-B08-213641	26133SI	40
Fagron	Prednisona	23A04-B03-226162	26618SI	40
Fagron	Prednisona	24A30-B09-237512	27373SI	40

- 201 315 spectra from a total of 4034 batches from further 842 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 104 spectra from 57 *Apo-Ident* customers from 59 batches from the substance/substance group *Prednisona*.
- Among them are spectra of independent samples from 58 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednisona	21003706007	1
	Prednisona	21003706008	1
Caelo	Prednisona	10037817	1
Caelo	Prednisona	10037826	1
Caelo	Prednisona	12177604	1
Caelo	Prednisona	12232705	3
Caelo	Prednisona	12232712	1
Caelo	Prednisona	12232713	1
Caelo	Prednisona	12232714	1
Caelo	Prednisona	13262302	1
Caelo	Prednisona	13262304	3
Caelo	Prednisona	15218602	5
Caelo	Prednisona	15218606	5
Caelo	Prednisona	15218607	1
Caelo	Prednisona	16277201	1
Caelo	Prednisona	16277206	1
Caelo	Prednisona	17166501	2
Caelo	Prednisona	17166502	5
Caelo	Prednisona	17166503	1
Caelo	Prednisona	17166504	1
Caelo	Prednisona	17166507	3
Caelo	Prednisona	17166508	2
Caelo	Prednisona	171666508	1
Caelo	Prednisona	18058701	1
Caelo	Prednisona	18108003	1
Caelo	Prednisona	18108004	2
Caelo	Prednisona	19245501	2
Caelo	Prednisona	19245502	1
Caelo	Prednisona	204312107	1
Caelo	Prednisona	21000576001	1
Caelo	Prednisona	21000576002	1
Caelo	Prednisona	21003706002	1
Caelo	Prednisona	21003706003	1
Caelo	Prednisona	21003706005	1
Caelo	Prednisona	21003706007	1
Caelo	Prednisona	2114Q2107	1
Caelo	Prednisona	28021401	1
Caelo	Prednisona	28021403	1
Caelo	Prednisona	5087	1
Caesar & Loretz GmbH...	Prednisona	18108004	1
Caesar & Loretz GmbH	Prednisona	17166508	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Prednisona	18108003	3
Caesar & Loretz GmbH	Prednisona	18108004	1
Caesar & Loretz GmbH	Prednisona	20001277001	1
Caesar & Loretz GmbH	Prednisona	21003706006	1
Euro OTC	Prednisona	1401042-02	1
Euro OTC	Prednisona	150043-03	1
Euro OTC	Prednisona	1501043-01	2
Euro OTC	Prednisona	1501043-02	1
Euro OTC	Prednisona	1501043-03	5
Euro OTC	Prednisona	1604051-01	3
Euro OTC	Prednisona	1604501-01	1
Euro OTC	Prednisona	1702008-01	3
Euro OTC	Prednisona	172008-01	1
Fagron	Prednisona	12E02-N01	1
Fagron	Prednisona	12E02-N10	1
Fagron	Prednisona	13C13-N08	1
Fagron	Prednisona	15218608	1
Fagron	Prednisona	16H04-B04-334368	1
Fagron	Prednisona	20F19-F02-371975	1
Fagron	Prednisona	21021401	1
Gehe	Prednisona	12232714	1
Gehe	Prednisona	12L14-M03	1
Gehe	Prednisona	13C13-N08	1
Gehe	Prednisona	17166508	1
Noweda	Prednisona	17166501	1
Noweda	Prednisona	17166503	1
Noweda	Prednisona	21003060027	1
Phönix	Prednisona	11D08-N05	1
sanacorp	Prednisona	13262302	1
Sanacorp	Prednisona	16277206	1

- 235 963 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	769	0	201 315
Type C	0	102	2	235 963

The substance/substance group *Prednisona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2198 %)
Type C	100.0000 % (> 99.9007 %)	98.0769 % (> 95.1923 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21408	22557	13,72	120,14
21409	22557	10,59	119,25
21573	21616	9,11	120,53
21616	21616	0,00	116,78
22557	22557	0,00	115,59
23227	24895	4,87	114,73
24895	24895	0,00	114,84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pregnenolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20721-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pregnenolona; Pregnenolonum

Special notes

When selecting the *Pregnenolona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pregnenolona	11	10	46

Second-stage model

For differentiation of the substance/substance group *Pregnenolona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pregnenolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prasterona	71,51	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pregnenolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pregnenolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Pregnenolona	1204040-01	20721	40	1404311
Euro OTC	Pregnenolona	1312007-01	21679	60	8985
Euro OTC	Pregnenolona	1602001	22375	45	20160208*
Euro OTC	Pregnenolona	1612019	22979	40	20170131*
Euro OTC	Pregnenolona	1908021	24849	40	20190913*
Euro OTC	Pregnenolona	1908020	24932	40	20191018*
Euro OTC	Pregnenolona	2006014	25325	40	20200803*
Euro OTC	Pregnenolona	2104008	25685	50	20210510*
Fagron	Pregnenolona	15B11-B07-310278	22355	45	9338
Fagron	Pregnenolona	18L27-B02-357840	24704	40	20190220
Fagron	Pregnenolona	22I19-B02	26445	40	20221201*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Pregnenolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 482 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 460 spectra of 13 reference samples from the substance/substance group *Pregnenolona*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Pregnenolona	1606028	22706	40
Euro OTC	Pregnenolona	1709017	23696	40
Euro OTC	Pregnenolona	1909013	24954	40
Euro OTC	Pregnenolona	2001037	25129	40
Euro OTC	Pregnenolona	2006015	25342	40
Euro OTC	Pregnenolona	2101012	25539	40
Euro OTC	Pregnenolona	2108003	25765	40
Euro OTC	Pregnenolona	2203003	26029	40
Euro OTC	Pregnenolona	2201037	26033	40
Fagron	Pregnenolona	23I28-B11-233503	27057	40
Euro OTC	Pregnenolona	2203003	26029SI	20
Euro OTC	Pregnenolona	2201037	26033SI	20
Fagron	Pregnenolona	23I28-B11-233503	27057SI	20

- 201 624 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 231 spectra from 24 *Apo-Ident* customers from 50 batches from the substance/substance group *Pregnenolona*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Pregnenolona	23D11-B02-226331	1
	Pregnenolona	23I28-B11-233501	1
	Pregnenolona	23I28-B11-233503	1
Audor Pharma	Pregnenolona	A141215/46	1
Audor Pharma	Pregnenolona	AP10L10-M01P	1
Audor Pharma	Pregnenolona	AP1109007-01P	1
Audor Pharma	Pregnenolona	APC07-150801(M)P	3
Audor Pharma	Pregnenolona	APC07-160801(M)P	2
Audor Pharma	Pregnenolona	APc07-180201	1
Audor Pharma	Pregnenolona	APC07-180201	2
Audor Pharma	Pregnenolona	APC07-180201(M)P	3
Audor Pharma	Pregnenolona	APc07-180702(M)-1P	1
Audor Pharma	Pregnenolona	APC07-180702(M)-1P	1
Audor Pharma	Pregnenolona	APC07-180702(M)-2P	1
bitte ergänzen	Pregnenolona		1
Euro OTC	Pregnenolona	1312007-01	1
Euro OTC	Pregnenolona	1402025-01	1
Euro OTC	Pregnenolona	1506002-01	10
Euro OTC	Pregnenolona	1602001-01	22
Euro OTC	Pregnenolona	1606028-01	29
Euro OTC	Pregnenolona	1612019-01	51
Euro OTC	Pregnenolona	1908021-01	2
Euro OTC	Pregnenolona	1908021-02	1
Euro OTC	Pregnenolona	2001037-01	24
Euro OTC	Pregnenolona	2001037-02	3
Euro OTC	Pregnenolona	2006015-01	5
Euro OTC	Pregnenolona	2006015-02	36
Euro OTC	Pregnenolona	2101012-01	2
Euro OTC	Pregnenolona	2108003-01	1
Euro OTC	Pregnenolona	2203003-01	2
Fagron	Pregnenolona	14B18-B04-291917	1
Fagron	Pregnenolona	16L29-B02331611	1
Fagron	Pregnenolona	19E01-B01-364473	1
Fagron	Pregnenolona	19J25-F02	1
Fagron	Pregnenolona	19J25-F02-367245	1
Fagron	Pregnenolona	19L09-F01-372068	1
Fagron	Pregnenolona	20104-F04-378102	1
Fagron	Pregnenolona	20I04-F04-374073	1
Fagron	Pregnenolona	23G20-B02-233060	1
Fagron	Pregnenolona	23I28-B11-233499	1
Fagron	Pregnenolona	F01-3720608	1
Fagron	Pregnenolona	F02-3672405	1
Fagron	Pregnenolona	F04-3784905	1
gehe	Pregnenolona	Apc07160801	1
Haihang Industry	Pregnenolona	20140329	1
Koisser Pharma	Pregnenolona	ZH-131001	1
Koisser	Pregnenolona	ZH-130802	1
KS Pharma	Pregnenolona	ZH-111119	1
NWM CHina	Pregnenolona	PR150329	1
NWM Shandong Northwe...	Pregnenolona	PRN151219	1

- 235 836 spectra from 1515 *Apo-Ident* customers from a total of 49 209 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pregnenolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pregnenolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	460	0	201 624
Type C	0	226	5	235 836

The substance/substance group *Pregnenolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6957 %)
Type C	100.0000 % (> 99.9007 %)	97.8355 % (> 96.5368 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20721	20721	0,00	92,66
21679	21679	0,00	92,42
22355	22355	0,00	97,80
22375	22375	0,00	92,67
22979	22979	0,00	93,73
24704	26445	7,28	96,69
24849	24849	0,00	93,05
24932	24932	0,00	96,87
25325	25325	0,00	96,73
25685	25685	0,00	98,15
26445	26445	0,00	95,59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prilocaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005414-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prilocaína

Special notes

When selecting the *Prilocaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prilocaína	2	1	0

Second-stage model

For differentiation of the substance/substance group *Prilocaína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prilocaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	121,97	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prilocaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prilocaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prilocaína	2208012	26336	40	20221018*
Euro OTC	Prilocaína	2310022	27370	40	20240826*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Prilocaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Prilocaína*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prilocaína	1909017-01	25782	50
Euro OTC	Prilocaína	2208012	26336SI†	20
Euro OTC	Prilocaína	2310022	27370SI†	20

- 201 994 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Prilocaína*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prilocaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

relevant spectra of the various substances were compared with *Prilocaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	87	3	201 994
Type C	0	0	0	236 067

The substance/substance group *Prilocaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	96.6667 % (> 93.3333 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26336	26336	0,00	197,90
27370	27370	0,00	200,10

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Progesterona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20024-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Progesterona; Progesteronum

Special notes

When selecting the *Progesterona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Progesterona	14	79	559

Second-stage model

For differentiation of the substance/substance group *Progesterona* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Progesterona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Espironolactona	61,73	58,50
⋮	⋮	⋮
Propionato de testosterona	>50	54,15
Povidona	>50	106,84
Ácido fusídico	>50	110,88
Iodopovidona	>50	123,57
Ubidecarenona	>50	127,08

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Progesterona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Progesterona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Progesterona	15319601	22831	40	20151014
Caelo	Progesterona	17060903	23249	40	20170315
Caelo	Progesterona	20002672	25658	50	20200914*
Caelo	Progesterona	20002672	25658SI	50	20200914*
Euro OTC	Progesterona	1111053-01	20718	30	20120119
Euro OTC	Progesterona	1506033	21868	60	0000010482
Euro OTC	Progesterona	1506033	21868SI	30	0000010482
Euro OTC	Progesterona	1506034	21870	60	0000010483
Euro OTC	Progesterona	1509008	21907	60	20150914*
Euro OTC	Progesterona	1511008	22226	60	20151119*
Euro OTC	Progesterona	1601009	22301	45	20160128*
Euro OTC	Progesterona	1601009	22301SI	45	20160128*
Euro OTC	Progesterona	1601001	22303	45	20160128*
Euro OTC	Progesterona	1603004	22525	40	20160406*
Euro OTC	Progesterona	2006018	25273	40	20200716*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Progesterona	2006018	25273SI	31	20200716*
Euro OTC	Progesterona	2103019	25684	50	20210427*
Euro OTC	Progesterona	2103019	25684SI	50	20210427*
Fagron	Progesterona	16A20-B02-319103	22830	40	20160209
Fagron	Progesterona	16A20-B02-319103	22830SI	40	20160209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 906 spectra of 20 reference samples from the substance/substance group *Progesterona*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.

- 152 056 spectra from a total of 2828 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 6386 spectra of 168 reference samples from the substance/substance group *Progesterona*.

- Among them are spectra of independent samples from 79 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Progesterona	170609	23329	40
Caelo	Progesterona	172778	23838	40
Caelo	Progesterona	191287	24750	40
Caelo	Progesterona	21002413	25792	40
Caelo	Progesterona	22001580	26252	40
Caelo	Progesterona	22001577	26256	40
Caelo	Progesterona	22003208	26485	40
Caelo	Progesterona	23003401	27104	40
Euro OTC	Progesterona	1603012	22529	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterona	1605013	22556	40
Euro OTC	Progesterona	1606033	22704	40
Euro OTC	Progesterona	1605032	22705	40
Euro OTC	Progesterona	1609016	22788	40
Euro OTC	Progesterona	1609001	22819	40
Euro OTC	Progesterona	1701038	23138	40
Euro OTC	Progesterona	1702026	23148	40
Euro OTC	Progesterona	1707012	23536	40
Euro OTC	Progesterona	1705028	23541	40
Euro OTC	Progesterona	1709012	23732	40
Euro OTC	Progesterona	1801036	23947	40
Euro OTC	Progesterona	1802030	24067	40
Euro OTC	Progesterona	1806020	24138	40
Euro OTC	Progesterona	1809018	24328	40
Euro OTC	Progesterona	1809017	24334	40
Euro OTC	Progesterona	1603012-01	24335	40
Euro OTC	Progesterona	1811033	24345	40
Euro OTC	Progesterona	1901021	24447	40
Euro OTC	Progesterona	1901022	24455	40
Euro OTC	Progesterona	1904033	24606	40
Euro OTC	Progesterona	1905023	24765	40
Euro OTC	Progesterona	1905022	24790	40
Euro OTC	Progesterona	1908002	24834	40
Euro OTC	Progesterona	1908003	24863	40
Euro OTC	Progesterona	1911006	24962	40
Euro OTC	Progesterona	1911007	24970	40
Euro OTC	Progesterona	2001036	25077	40
Euro OTC	Progesterona	2003037	25110	40
Euro OTC	Progesterona	2003042	25111	40
Euro OTC	Progesterona	2003036	25112	40
Euro OTC	Progesterona	2005019	25255	40
Euro OTC	Progesterona	2005018	25256	40
Euro OTC	Progesterona	2007029	25262	40
Euro OTC	Progesterona	2006017	25263	40
Euro OTC	Progesterona	2007028	25276	40
Euro OTC	Progesterona	2010005	25474	40
Euro OTC	Progesterona	2103020	25683	50
Euro OTC	Progesterona	2108010	25819	50
Euro OTC	Progesterona	2108011	25831	50
Euro OTC	Progesterona	2111009	25917	40
Euro OTC	Progesterona	2111008	25921	40
Euro OTC	Progesterona	2203007	26032	40
Euro OTC	Progesterona	2203006	26034	40
Euro OTC	Progesterona	2207002	26214	40
Euro OTC	Progesterona	2210017	26425	40
Euro OTC	Progesterona	2210016	26443	40
Euro OTC	Progesterona	2301049	26577	30
Euro OTC	Progesterona	2307007	26760	40
Euro OTC	Progesterona	2307006	26761	40
Euro OTC	Progesterona	2308001	26886	30
Euro OTC	Progesterona	2308002	26887	30
Euro OTC	Progesterona	2309026	26937	40
Euro OTC	Progesterona	2311009	27013	40
Euro OTC	Progesterona	2311010	27014	40
Euro OTC	Progesterona	2401013	27088	40
Euro OTC	Progesterona	2401014	27089	40
Euro OTC	Progesterona	2402023	27143	40
Euro OTC	Progesterona	2404001	27203	40
Euro OTC	Progesterona	2404005	27204	40
Euro OTC	Progesterona	2405006	27205	40

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterona	2405005	27208	40
Euro OTC	Progesterona	2406015	27284	40
Euro OTC	Progesterona	2406014	27285	40
Euro OTC	Progesterona	2407018	27354	40
Euro OTC	Progesterona	2407019	27355	30
Euro OTC	Progesterona	2409003	27398	40
Euro OTC	Progesterona	2410011	27461	40
Euro OTC	Progesterona	2410010	27462	40
Fagron	Progesterona	19H20-F02-364866	25046	40
Fagron	Progesterona	22H12-B01-222409	26407	40
Caelo	Progesterona	15319601	22831SI†	40
Caelo	Progesterona	17060903	23249SI†	20
Caelo	Progesterona	170609	23329SI	20
Caelo	Progesterona	172778	23838SI	30
Caelo	Progesterona	170609	23844	40
Caelo	Progesterona	170609	23844SI	23
Caelo	Progesterona	191287	24750SI	40
Caelo	Progesterona	21002413	25792SI	40
Caelo	Progesterona	22001580	26252SI	40
Caelo	Progesterona	22001577	26256SI	40
Caelo	Progesterona	22003208	26485SI	35
Caelo	Progesterona	23003401	27104SI	20
Euro OTC	Progesterona	1506033	21868SI†	20
Euro OTC	Progesterona	1506034	21870SI†	59
Euro OTC	Progesterona	1509008	21907SI†	53
Euro OTC	Progesterona	1511008	22226SI†	27
Euro OTC	Progesterona	1601001	22303SI†	44
Euro OTC	Progesterona	1603004	22525SI†	31
Euro OTC	Progesterona	1603012	22529SI	29
Euro OTC	Progesterona	1605013	22556SI	30
Euro OTC	Progesterona	1606033	22704SI	30
Euro OTC	Progesterona	1605032	22705SI	38
Euro OTC	Progesterona	1609016	22788SI	30
Euro OTC	Progesterona	1609001	22819SI	30
Euro OTC	Progesterona	1701038	23138SI	20
Euro OTC	Progesterona	1702026	23148SI	20
Euro OTC	Progesterona	1707012	23536SI	28
Euro OTC	Progesterona	1705028	23541SI	25
Euro OTC	Progesterona	1709012	23732SI	40
Euro OTC	Progesterona	1801036	23947SI	20
Euro OTC	Progesterona	1802030	24067SI	32
Euro OTC	Progesterona	1806020	24138SI	35
Euro OTC	Progesterona	1809018	24328SI	30
Euro OTC	Progesterona	1809017	24334SI	40
Euro OTC	Progesterona	1603012-01	24335SI	20
Euro OTC	Progesterona	1811033	24345SI	30
Euro OTC	Progesterona	1901021	24447SI	40
Euro OTC	Progesterona	1901022	24455SI	40
Euro OTC	Progesterona	1904033	24606SI	39
Euro OTC	Progesterona	1905023	24765SI	40
Euro OTC	Progesterona	1905022	24790SI	40
Euro OTC	Progesterona	1908002	24834SI	40
Euro OTC	Progesterona	1908003	24863SI	40
Euro OTC	Progesterona	1911006	24962SI	40
Euro OTC	Progesterona	1911007	24970SI	40
Euro OTC	Progesterona	2001036	25077SI	40
Euro OTC	Progesterona	2003037	25110SI	40
Euro OTC	Progesterona	2003042	25111SI	40
Euro OTC	Progesterona	2003036	25112SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterona	2005019	25255SI	30
Euro OTC	Progesterona	2005018	25256SI	40
Euro OTC	Progesterona	2007029	25262SI	39
Euro OTC	Progesterona	2006017	25263SI	40
Euro OTC	Progesterona	2007028	25276SI	40
Euro OTC	Progesterona	2010005	25474SI	40
Euro OTC	Progesterona	2103020	25683SI	50
Euro OTC	Progesterona	2108010	25819SI	50
Euro OTC	Progesterona	2108011	25831SI	50
Euro OTC	Progesterona	2111009	25917SI	40
Euro OTC	Progesterona	2111008	25921SI	40
Euro OTC	Progesterona	2203007	26032SI	40
Euro OTC	Progesterona	2203006	26034SI	40
Euro OTC	Progesterona	2207002	26214SI	40
Euro OTC	Progesterona	2210017	26425SI	40
Euro OTC	Progesterona	2210016	26443SI	40
Euro OTC	Progesterona	2301049	26577SI	40
Euro OTC	Progesterona	2307007	26760SI	40
Euro OTC	Progesterona	2307006	26761SI	40
Euro OTC	Progesterona	2308001	26886SI	31
Euro OTC	Progesterona	2308002	26887SI	31
Euro OTC	Progesterona	2309026	26937SI	40
Euro OTC	Progesterona	2311009	27013SI	35
Euro OTC	Progesterona	2311010	27014SI	40
Euro OTC	Progesterona	2401013	27088SI	35
Euro OTC	Progesterona	2401014	27089SI	40
Euro OTC	Progesterona	2402023	27143SI	40
Euro OTC	Progesterona	2404001	27203SI	38
Euro OTC	Progesterona	2404005	27204SI	35
Euro OTC	Progesterona	2405006	27205SI	39
Euro OTC	Progesterona	2405005	27208SI	40
Euro OTC	Progesterona	2406015	27284SI	40
Euro OTC	Progesterona	2406014	27285SI	36
Euro OTC	Progesterona	2407018	27354SI	40
Euro OTC	Progesterona	2407019	27355SI	39
Euro OTC	Progesterona	2409003	27398SI	40
Euro OTC	Progesterona	2410011	27461SI	30
Euro OTC	Progesterona	2410010	27462SI	40
Fagron	Progesterona	19H20-F02-364866	25046SI	40
Fagron	Progesterona	22H12-B01-222409	26407SI	40

- 195 698 spectra from a total of 3958 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3247 spectra from 474 *Apo-Ident* customers from 582 batches from the substance/substance group *Progesterona*.

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- Among them are spectra of independent samples from 558 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Progesterona	1401002-01	2
	Progesterona	14253906	1
	Progesterona	20F-F12-372268	1
	Progesterona	21001388011	2
	Progesterona	21001388017	1
	Progesterona	21001388020	1
	Progesterona	2108010-01	1
	Progesterona	22001580002	1
	Progesterona	22001580003	1
	Progesterona	22003208002	1
	Progesterona	22041400M	1
	Progesterona	2207002-01	2
	Progesterona	2210016-01	1
	Progesterona	22A31-F02-381709	1
	Progesterona	22A31-F02-381712	1
	Progesterona	22H12-B01-222409	3
	Progesterona	22H12-B01-222410	1
	Progesterona	22K17-B10-224492	1
	Progesterona	23002143002	1
	Progesterona	23002143003	5
	Progesterona	2301049-01	3
	Progesterona	2307006-01	1
	Progesterona	2307007-01	1
	Progesterona	2308001-01	1
	Progesterona	2309026-01	2
	Progesterona	2309026-02	2
	Progesterona	2311009-01	1
	Progesterona	23B08B03227299	1
	Progesterona	23B08-B03-227300	1
	Progesterona	23H07-B03-230995	1
	Progesterona	23H07-B04-230996	3
	Progesterona	23H07-B04-230997	4
	Progesterona	2401013-01	2
	Progesterona	2401013-02	1
	Progesterona	2404005-01	3
	Progesterona	2405005-01	1
	Progesterona	2406014-01	1
	Progesterona	C01-230408	1
	Progesterona	EU-HTT230308M	1
A.H. 03.06.13 ek: 6,50EUR	Progesterona	1304014-01	1
AHD	Progesterona	13I11-N11	1
Alliance Healthcare	Progesterona	1206024-02	1
Alliance	Progesterona	15i11-b05-315224	1
Alliance	Progesterona	15I11-B05-315224	2
Anzag 07.04.2016	Progesterona	APC01-150708P	1
ANZAG	Progesterona	12195907	2
Anzag	Progesterona	13K28-B01-293478	1
Anzag	Progesterona	14k11-b04-300921	1
Anzag	Progesterona	15C31-B06-312963	3
Anzag	Progesterona	2515A-03235	1
Audor Pharma	Progesterona	APC01-120613P	1
Audor Pharma	Progesterona	APC01-120708P	3
Audor Pharma	Progesterona	APC01-141212P	1
Audor Pharma	Progesterona	APC01-150311P	1
Audor Pharma	Progesterona	APC01-150708P	5
Audor Pharma	Progesterona	APC01-151114P	9
Audor Pharma	Progesterona	APC01-160201	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Progesterona	APC01-160201P	8
Audor Pharma	Progesterona	APC01-170828P	1
Audor Pharma	Progesterona	APC01-171101P	31
Audor Pharma	Progesterona	APC01-180128P	1
Audor Pharma	Progesterona	APC01-180610P	12
Audor Pharma	Progesterona	APC01-181003P	15
Audor Pharma	Progesterona	APC01-181003P	1
Audor Pharma	Progesterona	APOC01-1700828P	2
Audor Pharma	Progesterona	C01-120708P	1
Audor Pharma	Progesterona	C01-180128	10
cae	Progesterona	20004530001	1
Caelo	Progesterona	11177207	1
Caelo	Progesterona	11177219	3
Caelo	Progesterona	11177221	2
Caelo	Progesterona	117348404	1
Caelo	Progesterona	12195828	1
Caelo	Progesterona	12195902	1
Caelo	Progesterona	12195905	3
Caelo	Progesterona	12195906	4
Caelo	Progesterona	12195907	4
Caelo	Progesterona	12195912	3
Caelo	Progesterona	12195913	3
Caelo	Progesterona	12195914	3
Caelo	Progesterona	12195920	8
Caelo	Progesterona	12195924	10
Caelo	Progesterona	12195926	19
Caelo	Progesterona	12195928	7
Caelo	Progesterona	12A19-N04	2
Caelo	Progesterona	130404002	2
Caelo	Progesterona	13155902	10
Caelo	Progesterona	13155920	1
Caelo	Progesterona	13155921	2
Caelo	Progesterona	13155927	4
Caelo	Progesterona	13155928	3
Caelo	Progesterona	13155929	1
Caelo	Progesterona	13G11-N02	1
Caelo	Progesterona	13HI01-N03	1
Caelo	Progesterona	140100201	1
Caelo	Progesterona	14253911	6
Caelo	Progesterona	14253915	2
Caelo	Progesterona	14253929	1
Caelo	Progesterona	14253930	1
Caelo	Progesterona	14H13-B05-3002016	1
Caelo	Progesterona	14K11-B04-300920	2
Caelo	Progesterona	1511-B05-313598	1
Caelo	Progesterona	15124902	1
Caelo	Progesterona	15124910	4
Caelo	Progesterona	15124919	2
Caelo	Progesterona	15319601	7
Caelo	Progesterona	15319602	1
Caelo	Progesterona	15319603	42
Caelo	Progesterona	15319604	1
Caelo	Progesterona	15319607	3
Caelo	Progesterona	15319608	7
Caelo	Progesterona	15319618	4
Caelo	Progesterona	15319619	1
Caelo	Progesterona	15319620	1
Caelo	Progesterona	15C31-808	1
Caelo	Progesterona	15C31-B06-308796	2
Caelo	Progesterona	15I11-B05	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Progesterona	15I11-B05-314184	2
Caelo	Progesterona	160100902	1
Caelo	Progesterona	16015B14-315279	1
Caelo	Progesterona	1605013-02	1
Caelo	Progesterona	16103601	2
Caelo	Progesterona	16103602	4
Caelo	Progesterona	16103603	11
Caelo	Progesterona	16103604	1
Caelo	Progesterona	16103605	3
Caelo	Progesterona	16103606	12
Caelo	Progesterona	16103607	1
Caelo	Progesterona	16103609	30
Caelo	Progesterona	16103610	4
Caelo	Progesterona	16103613	20
Caelo	Progesterona	161036303	9
Caelo	Progesterona	16203605	1
Caelo	Progesterona	16A20-B02-319103	1
Caelo	Progesterona	16D13-B04	1
Caelo	Progesterona	16J05-B04-328263	1
Caelo	Progesterona	16L29-B03-330995	1
Caelo	Progesterona	17/21-B03-343284	1
Caelo	Progesterona	17060901	41
Caelo	Progesterona	17060903	6
Caelo	Progesterona	17060904	6
Caelo	Progesterona	17060905	2
Caelo	Progesterona	17060907	10
Caelo	Progesterona	17060909	13
Caelo	Progesterona	17060910	3
Caelo	Progesterona	17060911	2
Caelo	Progesterona	1706093	1
Caelo	Progesterona	17149903	1
Caelo	Progesterona	17149904	9
Caelo	Progesterona	17149905	1
Caelo	Progesterona	17149906	10
Caelo	Progesterona	17149907	1
Caelo	Progesterona	1719907	10
Caelo	Progesterona	1721bo3342134	1
Caelo	Progesterona	17277801	22
Caelo	Progesterona	1734801	1
Caelo	Progesterona	1734804	2
Caelo	Progesterona	17348401	2
Caelo	Progesterona	17348402	6
Caelo	Progesterona	17348403	10
Caelo	Progesterona	17348404	13
Caelo	Progesterona	17348405	3
Caelo	Progesterona	17348407	7
Caelo	Progesterona	17348409	5
Caelo	Progesterona	1760911	1
Caelo	Progesterona	17C15-B03-333671	1
Caelo	Progesterona	17I21-B03-342136	1
Caelo	Progesterona	1801036-01	16
Caelo	Progesterona	18098801	25
Caelo	Progesterona	182632802	1
Caelo	Progesterona	1826380	1
Caelo	Progesterona	182638004	5
Caelo	Progesterona	182638005	5
Caelo	Progesterona	182638009	1
Caelo	Progesterona	18263801	3
Caelo	Progesterona	182638010	16
Caelo	Progesterona	18263802	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Progesterona	18263804	15
Caelo	Progesterona	18263807	4
Caelo	Progesterona	18263809	9
Caelo	Progesterona	18263811	1
Caelo	Progesterona	18B06-B10	3
Caelo	Progesterona	18B06-B10-346702	1
Caelo	Progesterona	18F22-B04-351435	1
Caelo	Progesterona	18f22-B04-354899	1
Caelo	Progesterona	18F22-B04-355395	1
Caelo	Progesterona	19000591002	13
Caelo	Progesterona	19000591005	7
Caelo	Progesterona	19051502	1
Caelo	Progesterona	19128702	1
Caelo	Progesterona	19128705	2
Caelo	Progesterona	19A25-B01-360450	1
Caelo	Progesterona	20004178001	1
Caelo	Progesterona	20004179001	5
Caelo	Progesterona	20004530002	6
Caelo	Progesterona	20004530003	2
Caelo	Progesterona	200303701	1
Caelo	Progesterona	2005019-01	1
Caelo	Progesterona	2006500002	1
Caelo	Progesterona	21001388	1
Caelo	Progesterona	21001388001	1
Caelo	Progesterona	21001388003	6
Caelo	Progesterona	21001388007	2
Caelo	Progesterona	21001388008	1
Caelo	Progesterona	21001388010	2
Caelo	Progesterona	21001388020	3
Caelo	Progesterona	2100138804	1
Caelo	Progesterona	21002413001	1
Caelo	Progesterona	258/61	1
Caelo	Progesterona	27121303	1
Caelo	Progesterona	4814A-03235	1
Caelo	Progesterona	4817Q-03235	1
Caelo	Progesterona	7101401	1
Caelo	Progesterona	9031705	1
Caelo	Progesterona	9195408	1
Caelo	Progesterona	9195429	1
Caelo	Progesterona	B03333671	1
Caelo	Progesterona	C01-120613	1
Caelo	Progesterona	EU-HTT160708	1
Caelo	Progesterona	EU-HTT180317	1
Caelo	Progesterona	HTT140302	1
Caeolo/Gehe	Progesterona	17060903	2
Caesar & Loretz GmbH...	Progesterona	18263804	1
Caesar & Loretz GmbH...	Progesterona	21001388003	1
Caesar & Loretz GmbH...	Progesterona	182638010	1
Caesar & Loretz GmbH...	Progesterona	21001388003	1
Caesar & Loretz GmbH/Gehe	Progesterona	18263801	1
Caesar & Loretz GmbH/Gehe	Progesterona	18263809	1
Caesar & Loretz GmbH...	Progesterona	18263804	1
Caesar & Loretz GmbH...	Progesterona	18263804	1
Caesar & Loretz GmbH...	Progesterona	18263809	2
Caesar & Loretz GmbH...	Progesterona	19128705	4
Caesar & Loretz GmbH...	Progesterona	20004530002	1
Caesar & Loretz GmbH/phö	Progesterona	182638004	1
Caesar & Loretz GmbH...	Progesterona	21001388003	1
Caesar & Loretz GmbH	Progesterona	17060910	1
Caesar & Loretz GmbH	Progesterona	17348404	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Progesterona	17348405	1
Caesar & Loretz GmbH	Progesterona	17348409	2
Caesar & Loretz GmbH	Progesterona	182638004	5
Caesar & Loretz GmbH	Progesterona	182638010	9
Caesar & Loretz GmbH	Progesterona	18263804	6
Caesar & Loretz GmbH	Progesterona	18263807	3
Caesar & Loretz GmbH	Progesterona	18263809	5
Caesar & Loretz GmbH	Progesterona	20004530002	4
Caesar & Loretz GmbH	Progesterona	2007029-01	1
Caesar & Loretz GmbH	Progesterona	21001388001	3
Caesar & Loretz GmbH	Progesterona	21001388003	2
Caesar & Loretz GmbH	Progesterona	21001388004	4
Caesar & Loretz GmbH	Progesterona	21001388007	2
Caesar & Loretz GmbH	Progesterona	21001388011	1
Caesar & Loretz GmbH	Progesterona	22001580001	3
Caesar & Loretz GmbH	Progesterona	23002143003	1
Caesar & Loretz GmbH	Progesterona	EUHTT190101	1
Caesar & Loretz/Geil...	Progesterona	17060904	1
Caesar & Loretz/Noweda	Progesterona	19000591004	3
Caesar u Loretz	Progesterona	13155920	1
Caesar u Loretz	Progesterona	15124919	1
Caesar&Lorenz	Progesterona	16103605	1
Caesar/Noweda	Progesterona	12195912	1
Cealo/Noweda	Progesterona	16103607	1
Changzhou Jiaerke Pharma	Progesterona	1308015-01	1
China Medica	Progesterona	1308015-01	1
Ebert u. Jacobi 1...	Progesterona	15C31-B06-312963	1
Ebert-Jacobi	Progesterona	16J05-B04-328263	1
EuRho/EuRho	Progesterona	1904033-01	1
EuRho	Progesterona	1304040-02	1
euRho	Progesterona	2103020-01	1
EuRho	Progesterona	2203007-01	1
Euro OTC	Progesterona		2
Euro OTC	Progesterona	1111053-01	6
Euro OTC	Progesterona	1206024-01	1
Euro OTC	Progesterona	1211004-01	5
Euro OTC	Progesterona	12195924	1
Euro OTC	Progesterona	130404001	1
Euro OTC	Progesterona	1304040-01	4
Euro OTC	Progesterona	1304040-02	3
Euro OTC	Progesterona	1308015-01	3
Euro OTC	Progesterona	1401002-01	3
Euro OTC	Progesterona	1403019-01	2
Euro OTC	Progesterona	1406022-01	1
Euro OTC	Progesterona	140602202	1
Euro OTC	Progesterona	1406022-02	2
Euro OTC	Progesterona	1406910-01	1
Euro OTC	Progesterona	1409019-01	1
Euro OTC	Progesterona	1409029-01	6
Euro OTC	Progesterona	1409029-1	1
Euro OTC	Progesterona	140910-01	1
Euro OTC	Progesterona	141104301	1
Euro OTC	Progesterona	1411043-01	4
Euro OTC	Progesterona	15/11-B05-315224	1
Euro OTC	Progesterona	1502030-01	2
Euro OTC	Progesterona	1503012-01	7
Euro OTC	Progesterona	1503033-01	1
Euro OTC	Progesterona	1506033-01	51
Euro OTC	Progesterona	1509008_01	1
Euro OTC	Progesterona	1509008-01	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Progesterona	1509008-02	31
Euro OTC	Progesterona	160100901	1
Euro OTC	Progesterona	1601009-01	55
Euro OTC	Progesterona	1601009-02	52
Euro OTC	Progesterona	1603004-01	46
Euro OTC	Progesterona	1603012-01	1
Euro OTC	Progesterona	1605013-01	35
Euro OTC	Progesterona	1605013-02	45
Euro OTC	Progesterona	160501303	2
Euro OTC	Progesterona	1605013-03	6
Euro OTC	Progesterona	1605032-01	46
Euro OTC	Progesterona	160532-01	15
Euro OTC	Progesterona	1609001-01	65
Euro OTC	Progesterona	1701038-01	30
Euro OTC	Progesterona	170103802	9
Euro OTC	Progesterona	1701038-02	33
Euro OTC	Progesterona	170138-01	20
Euro OTC	Progesterona	1704012-01	8
Euro OTC	Progesterona	1705028	1
Euro OTC	Progesterona	170502801	1
Euro OTC	Progesterona	1705028-01	64
Euro OTC	Progesterona	1706009-01	9
Euro OTC	Progesterona	1709012-01	100
Euro OTC	Progesterona	17I08-B04	1
Euro OTC	Progesterona	1801036-01	11
Euro OTC	Progesterona	1801036-02	16
Euro OTC	Progesterona	18041816	1
Euro OTC	Progesterona	1806020-01	55
Euro OTC	Progesterona	1806020-02	1
Euro OTC	Progesterona	180901701	20
Euro OTC	Progesterona	1809017-01	62
Euro OTC	Progesterona	1809017-02	1
Euro OTC	Progesterona	1809018-02	1
Euro OTC	Progesterona	1811033-01	64
Euro OTC	Progesterona	1901021-01	3
Euro OTC	Progesterona	1901022-01	36
Euro OTC	Progesterona	1904033_01	1
Euro OTC	Progesterona	1904033-01	6
Euro OTC	Progesterona	190433-01	1
Euro OTC	Progesterona	1905022-01	4
Euro OTC	Progesterona	1905023-01	3
Euro OTC	Progesterona	1908002-01	12
Euro OTC	Progesterona	1908003-01	3
Euro OTC	Progesterona	1911006-01	1
Euro OTC	Progesterona	1911007-01	38
Euro OTC	Progesterona	19A25-B01-360449	1
Euro OTC	Progesterona	2001036-01	1
Euro OTC	Progesterona	2003036-01	2
Euro OTC	Progesterona	2003037-01	1
Euro OTC	Progesterona	2003042	2
Euro OTC	Progesterona	200304201	2
Euro OTC	Progesterona	2003042-01	1
Euro OTC	Progesterona	2005018-01	4
Euro OTC	Progesterona	2005019-01	19
Euro OTC	Progesterona	2006017-02	3
Euro OTC	Progesterona	2006018-01	95
Euro OTC	Progesterona	200618-01	1
Euro OTC	Progesterona	2007028-02	3
Euro OTC	Progesterona	2007029-01	122
Euro OTC	Progesterona	2010005-01	56

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Progesterona	2103019-01	3
Euro OTC	Progesterona	2103020-01	106
Euro OTC	Progesterona	210801001	1
Euro OTC	Progesterona	2108010-01	97
Euro OTC	Progesterona	2108011-01	3
Euro OTC	Progesterona	2111008-01	3
Euro OTC	Progesterona	2111009-01	5
Euro OTC	Progesterona	2203006-01	3
Euro OTC	Progesterona	2203007-01	7
Euro OTC	Progesterona	2210016-01	1
Euro OTC	Progesterona	2210017	1
Euro OTC	Progesterona	2210017-01	1
Euro OTC	Progesterona	27061713	1
Euro OTC	Progesterona	5102	1
Euro OTC	Progesterona	5104	1
Euro OTC	Progesterona	7406022-01	1
Euro OTC	Progesterona	818A-03235	1
Euro OTC	Progesterona	c01-111218	1
Euro OTC	Progesterona	c01-130301	1
Euro OTC	Progesterona	C01-130301(M)	2
Euro OTC	Progesterona	C01-130301M	1
Euro OTC	Progesterona	co1-111218(M)	1
Euro OTC	Progesterona	EuroOTC	1
Euro OTC	Progesterona	HTT160102	1
Euro/ Sanacorp	Progesterona	C01-131116(M)	1
EURO/Noweda	Progesterona	191100701	1
EURO/Noweda	Progesterona	200304201	1
Euro	Progesterona	1509008-02	1
Europh-Jenne	Progesterona	1406022-01	1
Fagron	Progesterona		2
Fagron	Progesterona	1-111218	1
Fagron	Progesterona	12A19-N04	1
Fagron	Progesterona	12D05-N06	3
Fagron	Progesterona	12G05-N17	6
Fagron	Progesterona	12K05-N01	2
Fagron	Progesterona	12k05-n07	1
Fagron	Progesterona	12K05-N07	1
Fagron	Progesterona	13/11-N11	1
Fagron	Progesterona	1311-N11	1
Fagron	Progesterona	13A02N01	1
Fagron	Progesterona	13A02-N01	3
Fagron	Progesterona	13AC2-N01	1
Fagron	Progesterona	13b08-n01	1
Fagron	Progesterona	13G11-N02	6
Fagron	Progesterona	13h01-n03	1
Fagron	Progesterona	13H01-N03	7
Fagron	Progesterona	13I11-N11	2
Fagron	Progesterona	13k28-b30-288261	1
Fagron	Progesterona	13K28-B30-288261	1
Fagron	Progesterona	13K28-B30-288262	1
Fagron	Progesterona	13K-B30-288261	1
Fagron	Progesterona	14C10-B01	1
Fagron	Progesterona	14C10B0129347	1
Fagron	Progesterona	14c10-b01-293478	1
Fagron	Progesterona	14c10-B01-293478	1
Fagron	Progesterona	14C10-B01-293478	2
Fagron	Progesterona	14D22-B04	2
Fagron	Progesterona	14D22B04293476	1
Fagron	Progesterona	14D22-B04-293476	2
Fagron	Progesterona	14D22-B04-293477	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterona	14D22-B293479	1
Fagron	Progesterona	14D22-Bo4	1
Fagron	Progesterona	14H13-B05-300216	7
Fagron	Progesterona	14k11-b04	1
Fagron	Progesterona	14K11-B04	3
Fagron	Progesterona	14K11-B04_300921	1
Fagron	Progesterona	14K11-B04-3000920	1
Fagron	Progesterona	14K11B04300920	1
Fagron	Progesterona	14K11-B04-300920	6
Fagron	Progesterona	14K11-B04-300921	3
Fagron	Progesterona	14L15-B05-302292	2
Fagron	Progesterona	14O22-B04-293476	1
Fagron	Progesterona	15/11-B05-315224	3
Fagron	Progesterona	1511-805	1
Fagron	Progesterona	1511-B05-313598	2
Fagron	Progesterona	1511-B05-313598GB	1
Fagron	Progesterona	1511-B05-314184	1
Fagron	Progesterona	1511-B05-314842	1
Fagron	Progesterona	1511B05-315224	1
Fagron	Progesterona	15B12-B04-304837	2
Fagron	Progesterona	15B12-Bo4-304838	1
Fagron	Progesterona	15C31-B06	3
Fagron	Progesterona	15C31B06308439	1
Fagron	Progesterona	15C31-B06-308439	7
Fagron	Progesterona	15C31-B06-308786	1
Fagron	Progesterona	15C31-B06-308796	4
Fagron	Progesterona	15C31-B06-309790	3
Fagron	Progesterona	15C31-B06-312963	1
Fagron	Progesterona	15C31-B06-313599	1
Fagron	Progesterona	15C31-B06-316105	3
Fagron	Progesterona	15C31-Bo6-308796	1
Fagron	Progesterona	15I11-B05	1
Fagron	Progesterona	15I11-B05-313598	2
Fagron	Progesterona	15I11-B05-314184	4
Fagron	Progesterona	15I11-B05-314842	1
Fagron	Progesterona	15I11-B05-315224	3
Fagron	Progesterona	1605013-03	1
Fagron	Progesterona	160A20-B02-321373	1
Fagron	Progesterona	16a20-b02-318667	1
Fagron	Progesterona	16A20-B02-318667	3
Fagron	Progesterona	16A20-B02-318668	1
Fagron	Progesterona	16A20-B02-319103	2
Fagron	Progesterona	16A20-B02-321373	2
Fagron	Progesterona	16A20-B02-321374	4
Fagron	Progesterona	16a20-b02-321375	1
Fagron	Progesterona	16A20-B02-321375	2
Fagron	Progesterona	16D13-B04-323636	1
Fagron	Progesterona	16g115-b04-325136	1
Fagron	Progesterona	16g15-b04	1
Fagron	Progesterona	16G15-B04	2
Fagron	Progesterona	16G15-B04-325135	1
Fagron	Progesterona	16G15-B04325136	1
Fagron	Progesterona	16G15-B04-325136	4
Fagron	Progesterona	16G15B04-325279	1
Fagron	Progesterona	16G15-B04325279	1
Fagron	Progesterona	16G15-B04-325279	6
Fagron	Progesterona	16G15-B04-325755	4
Fagron	Progesterona	16G15-B04-32579	1
Fagron	Progesterona	16g15-b04-326487	1
Fagron	Progesterona	16G15-B04-326487	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterona	16J05-B04-328263	3
Fagron	Progesterona	16J05-B04-328303	3
Fagron	Progesterona	16l11-B04-314184	1
Fagron	Progesterona	16L29-B03	1
Fagron	Progesterona	16L29-B03-302060	1
Fagron	Progesterona	16L29-B03-330995	2
Fagron	Progesterona	16l29b03332060	1
Fagron	Progesterona	16L29-B03-332060	5
Fagron	Progesterona	16L29-B03-332505	4
Fagron	Progesterona	16L29-B-332061	1
Fagron	Progesterona	17/21-B03-341517	1
Fagron	Progesterona	17/21-B03-341518	1
Fagron	Progesterona	17/21-B03-342134	2
Fagron	Progesterona	17/21-B03-342135	2
Fagron	Progesterona	17/21-B03-343284	2
Fagron	Progesterona	17060911	1
Fagron	Progesterona	1721B03342134	1
Fagron	Progesterona	1721-B03-342136	1
Fagron	Progesterona	17C15-B03	1
Fagron	Progesterona	17C15B03333671	2
Fagron	Progesterona	17C15-B03-333671	3
Fagron	Progesterona	17C15-B03-333671	1
Fagron	Progesterona	17C15-B03-333672	2
Fagron	Progesterona	17d25-b06	1
Fagron	Progesterona	17D25-B06-339651	3
Fagron	Progesterona	17D25-B06-339655	2
Fagron	Progesterona	17I08-B04	1
Fagron	Progesterona	17I08-B04-344773	1
Fagron	Progesterona	17I21-803	1
Fagron	Progesterona	17I21-B03	1
Fagron	Progesterona	17I21-B03-341516	2
Fagron	Progesterona	17I21-B03-341518	2
Fagron	Progesterona	17I21-B03-341520	3
Fagron	Progesterona	17I21-B03-342135	1
Fagron	Progesterona	17I21-B03-343284	2
Fagron	Progesterona	18806-B10-349153	1
Fagron	Progesterona	18B06_B10_349775	1
Fagron	Progesterona	18B06-B10	5
Fagron	Progesterona	18B06-B10-346701	5
Fagron	Progesterona	18B06-B10-346702	2
Fagron	Progesterona	18B06-B10-346704	4
Fagron	Progesterona	18B06B10347484	1
Fagron	Progesterona	18B06-B10-347484	4
Fagron	Progesterona	18B06-B10-349153	1
Fagron	Progesterona	18B06-B10-349775	3
Fagron	Progesterona	18F22_B04_354899	1
Fagron	Progesterona	18F22-B04	5
Fagron	Progesterona	18F-22-B04	1
Fagron	Progesterona	18F22-B04-351145	3
Fagron	Progesterona	18F22-B04-351435	3
Fagron	Progesterona	18F22-B04-351998	2
Fagron	Progesterona	18F22-B04-352735	3
Fagron	Progesterona	18F22-B04-352736	1
Fagron	Progesterona	18f22-B04-353582	1
Fagron	Progesterona	18F22-B04-353582	2
Fagron	Progesterona	18F22-B04353582-P201	1
Fagron	Progesterona	18F22-B04-354899	3
Fagron	Progesterona	18F22-B04-354900	4
Fagron	Progesterona	18F22-B04-354901	2
Fagron	Progesterona	18F22-B04-355395	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterona	18F22-HTT180317	1
Fagron	Progesterona	1910213235	1
Fagron	Progesterona	19A25-B01	1
Fagron	Progesterona	19A25-B01-360448	1
Fagron	Progesterona	19A25-B01-360449	8
Fagron	Progesterona	19A25-B01-360450	1
Fagron	Progesterona	19A25-B01-360452	1
Fagron	Progesterona	19A25-B01-360458	3
Fagron	Progesterona	19H20-F02	9
Fagron	Progesterona	19H20-F02-364866	3
Fagron	Progesterona	19H20-F02-364867	2
Fagron	Progesterona	19H20-F02-364868	4
Fagron	Progesterona	19H20-F02-364869	2
Fagron	Progesterona	19H20-F02-364870	2
Fagron	Progesterona	19H20-F02-364871	1
Fagron	Progesterona	19H2O-FO2-364866	1
Fagron	Progesterona	19J22-F05	2
Fagron	Progesterona	19J22-F05-3655503	1
Fagron	Progesterona	19J22F05-365551	1
Fagron	Progesterona	19J22-F05-365551	3
Fagron	Progesterona	19J22-F05-365552	4
Fagron	Progesterona	19J22-F05-365553	7
Fagron	Progesterona	19J22-F05-365555	1
Fagron	Progesterona	19J22-F05-365556	2
Fagron	Progesterona	19K11-F04	3
Fagron	Progesterona	19K11-F04-3660209	1
Fagron	Progesterona	19K11-F04-366029	2
Fagron	Progesterona	19K11-F04-366031	1
Fagron	Progesterona	19K11-F04-366033	2
Fagron	Progesterona	200650-0003	1
Fagron	Progesterona	200650-0004	2
Fagron	Progesterona	200650-315224	1
Fagron	Progesterona	20103-F01-374019	1
Fagron	Progesterona	20103-F01-374023	1
Fagron	Progesterona	20103-F01-375531	1
Fagron	Progesterona	20170427Ma6	1
Fagron	Progesterona	20F18-F12	3
Fagron	Progesterona	20F18-F12-32269	1
Fagron	Progesterona	20F18-F12-3722607	1
Fagron	Progesterona	20F18-F12-372267	3
Fagron	Progesterona	20F18-F12-372268	2
Fagron	Progesterona	20F18-f12-372269	1
Fagron	Progesterona	20F18-F12-372269	1
Fagron	Progesterona	20F18-F12-372270	9
Fagron	Progesterona	20F18-F12-372271	1
Fagron	Progesterona	20F18-F12-372272	6
Fagron	Progesterona	20F18-F12-372274	1
Fagron	Progesterona	20F18-F12-372275	3
Fagron	Progesterona	20I03-F01-374018	4
Fagron	Progesterona	20I03-F01-374019	2
Fagron	Progesterona	20I03-F01-374023	2
Fagron	Progesterona	20i03F01375531	1
Fagron	Progesterona	20I03-F01-375531	1
Fagron	Progesterona	21E11-F01	1
Fagron	Progesterona	21E11-F01-378406	2
Fagron	Progesterona	21F01-F02-378515	1
Fagron	Progesterona	21G14F04	1
Fagron	Progesterona	21G14-F04	2
Fagron	Progesterona	21G14-F04-379182	4
Fagron	Progesterona	21G14-F04-379183	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterona	21G14-F04-379607	2
Fagron	Progesterona	21G14-F04-379608	1
Fagron	Progesterona	21G14-F04-381038	1
Fagron	Progesterona	21G14-FO4-379607	1
Fagron	Progesterona	22A31-F02	1
Fagron	Progesterona	22A31-F02-381709	1
Fagron	Progesterona	22A31-F02-381711	2
Fagron	Progesterona	22A31-F02-381712	1
Fagron	Progesterona	22A31-F02-381713	1
Fagron	Progesterona	22A31-F02-381714	5
Fagron	Progesterona	22D05-F03-382185	1
Fagron	Progesterona	22H12-B01	4
Fagron	Progesterona	22H12-B02-226405	1
Fagron	Progesterona	22H12-Bo1	1
Fagron	Progesterona	23B08_B03_227303	1
Fagron	Progesterona	23B08-B03-227300	1
Fagron	Progesterona	23B08-B03-227303	2
Fagron	Progesterona	23H07-B04-232935	1
Fagron	Progesterona	375779	1
Fagron	Progesterona	5013I-03235	1
Fagron	Progesterona	ApC01-180128P	1
Fagron	Progesterona	C01-120322	1
Fagron	Progesterona	C01-130301	1
Fagron	Progesterona	C01-170814	1
Fagron	Progesterona	C01-171216	1
Fagron	Progesterona	EU_HTT190405	1
Fagron	Progesterona	EU-HTT160502	1
Fagron	Progesterona	EU-HTT160705	2
Fagron	Progesterona	EU-HTT180317	1
Fagron	Progesterona	EU-HTT190101	1
Fagron	Progesterona	EU-HTT190405	1
Fagron	Progesterona	EU-HTT200401	3
Fagron	Progesterona	EU-HTT220202M	1
Fagron	Progesterona	EU-HTT220316M	1
Fagron	Progesterona	F01-3740202	1
Fagron	Progesterona	F01-3740203	2
Fagron	Progesterona	F01-3755301	1
Fagron	Progesterona	F02-3648606	1
Fagron	Progesterona	F05_3655501	1
Fagron	Progesterona	F05-3655505	1
Fagron	Progesterona	F12-3722607	3
Fagron	Progesterona	F12-3722609	2
Fagron	Progesterona	F12-3722700	1
Fagron	Progesterona	F12-3722702	1
Fagron	Progesterona	F12-3722704	2
Fagron	Progesterona	F12-372271	1
Fagron	Progesterona	HTT140207	1
Fagron	Progesterona	HTT140302	1
Fagron	Progesterona	HTT140413	1
Fagron	Progesterona	HTT140503	1
Fagron	Progesterona	HTT140903	1
Fagron	Progesterona	HTT150201	3
Fagron	Progesterona	intern20180619Ma3	1
Fargon	Progesterona	16L29-B03-332505	1
fargon	Progesterona	18I03-B02-355396	1
Fargon	Progesterona	19J22-F-05-365555	1
Fiebig	Progesterona	17060909	1
Fiebig	Progesterona	17I21-B03	1
Fragon	Progesterona	13A02-N02	1
fragron	Progesterona	16A20-B02-319103	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Progesterona	15319608	1
Gehe	Progesterona	17060903	1
Gehe	Progesterona	18B06-B10-347484	1
Gehe	Progesterona	2309026-02	1
Geilenkirchen	Progesterona	16103605	1
Geilenkirchen	Progesterona	16103614	1
Geilenkirchen	Progesterona	17060904	2
Geilenkirchen	Progesterona	17060909	1
Geilenkirchen	Progesterona	17348407	2
Hubei Gedian Humanwell	Progesterona	EU-HTT200401	1
keine Angabe	Progesterona	1304040-01	2
Klenk	Progesterona	C01-120322	1
Kögl	Progesterona	1802398	1
L12	Progesterona	1605013-01	1
L12	Progesterona	17060909	2
L30	Progesterona	17060910	1
L30	Progesterona	18B06-B10-349775	1
Muster	Progesterona	HTT150801	1
Muster	Progesterona	HTT151101	1
Noweda	Progesterona	18B06-B10-349775	1
Noweda	Progesterona	19K11-F04-366029	1
Noweda	Progesterona	23002143004	1
Noweda	Progesterona	F04-3660209	1
Parthe Apotheke	Progesterona	71/21	1
PHOENIX am 18.03.2014	Progesterona	13A02-N01	1
Phoenix 09.12.14	Progesterona	13H01-N03	1
Phoenix 28.03.2014	Progesterona	13G11-N02	1
Phoenix/Cealo	Progesterona	17/21-B03-341517	1
Phoenix	Progesterona	20F18-F12	1
Phoenix	Progesterona	20F18-F12-372270	1
Phoenix	Progesterona	EU-HTT190405	1
Phönix	Progesterona	13155920	1
Phönix	Progesterona	15319604	1
Phönix	Progesterona	15319620	1
Phönix	Progesterona	1605013-01	1
Phönix	Progesterona	16A20-B02-319103	1
Phönix	Progesterona	16G15-B04_325135	1
phönix	Progesterona	16g15-b04-326487	1
Phönix	Progesterona	2003042-01	1
phönix	Progesterona	20F18-F12-372269	1
Phönix	Progesterona	20F18-F12-372269	1
Phönix	Progesterona	21E11-F013778406	1
Phönix	Progesterona	23002143003	1
Sanacorp Verbund	Progesterona	20I03-F01-374020	1
Sanacorp/Caesar & Lo…	Progesterona	21001388003	2
Sanacorp	Progesterona	12195914	1
Sanacorp	Progesterona	12195928	1
Sanacorp	Progesterona	13155902	1
Sanacorp	Progesterona	13A02-N01	1
Sanacorp	Progesterona	14C10-B01-293478	1
Sanacorp	Progesterona	15/11-B05-315224	3
sanacorp	Progesterona	15124902	1
Sanacorp	Progesterona	17D25-B06	1
Sanacorp	Progesterona	1809017-01	1
Sanacorp	Progesterona	19H20-F02-364869	1
Sanacorp	Progesterona	19J22-F05	1
Sanacorp	Progesterona	2007029-01	1
Sanacorp	Progesterona	20F18-F12	2
Sanacorp	Progesterona	21001388015	1
Sanacorp	Progesterona	2111009-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Progesterona	23002143003	1
Sanacorp	Progesterona	23H07-B03-230995	1
unbekannt	Progesterona	104704	1
Vdl 28.04.14;Preis 39,95	Progesterona		1
VDL;07.11.14;39,95 euro	Progesterona	13155921	1

- 232 820 spectra from 1515 *Apo-Ident* customers from a total of 48 680 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Progesterona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Progesterona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	906	0	152 056
Type B	0	6386	0	195 698
Type C	0	3201	46	232 820

The substance/substance group *Progesterona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3377 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.9060 %)
Type C	100.0000 % (> 99.9007 %)	98.5833 % (> 98.4909 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20718	22303	5,19	67,83
21868	21868	0,00	75,89
21870	21870	0,00	72,99
21907	21907	0,00	74,86
22226	22226	0,00	68,88
22301	22301	0,00	76,95
22303	22303	0,00	71,97
22525	22525	0,00	83,57
22830	21907	3,67	83,57
22831	22303	3,75	76,05
23249	22303	5,56	71,74
25273	25273	0,00	71,02
25658	25658	0,00	73,24
25684	25684	0,00	76,02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prolina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21034-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prolina; Prolinum

Special notes

When selecting the *Prolina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prolina	9	4	2

Second-stage model

For differentiation of the substance/substance group *Prolina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prolina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	82,56	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prolina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prolina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prolina	1606010	22677	40	20160714*
Euro OTC	Prolina	1705021	23546	40	20170720*
Euro OTC	Prolina	1801047	23961	40	20180206*
Euro OTC	Prolina	2009012	25418	40	20200928*
Euro OTC	Prolina	2111021	25916	40	20220112*
Euro OTC	Prolina	2205012	26210	40	20220608*
Euro OTC	Prolina	2205012	26210SI	20	20220608*
Euro OTC	Prolina	2308005	26870	40	20230824*
Euro OTC	Prolina	2308005	26870SI	20	20230824*
Fagron	Prolina	15D13-B02-308152	22270	60	1704059
Fagron	Prolina	16J14-B01-327195	23109	40	20161116

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 420 spectra of 11 reference samples from the substance/substance group *Prolina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 6 reference samples from the substance/substance group *Prolina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prolina	L1210046-01	21103	40
Euro OTC	Prolina	1606010-01	23013	40
Euro OTC	Prolina	1812009	24419	40
Euro OTC	Prolina	1909002	24844	40
Euro OTC	Prolina	1606010-01	23100	40
Euro OTC	Prolina	2111021	25916SI†	10

- 201 874 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Prolina*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Euro OTC	Prolina	L1210046-03	1
Fagron	Prolina	20J01-F13-374496	1

- 236 065 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prolina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prolina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	210	0	201 874
Type C	0	2	0	236 065

The substance/substance group *Prolina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9013 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22270	22270	0,00	217,10
22677	22677	0,00	176,08
23109	22270	4,64	216,08
23546	23546	0,00	186,65

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23961	23961	0,00	207,89
25418	25418	0,00	216,53
25916	25916	0,00	215,43
26210	26210	0,00	212,72
26870	26870	0,00	212,18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Propifenazona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20805-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propifenazona; Propyphenazonum

Special notes

When selecting the *Propifenazona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Propifenazona	6	4	36

Second-stage model

For differentiation of the substance/substance group *Propifenazona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Propifenazona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Griseofulvina	86,72	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Propifenazona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Propifenazona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propifenazona	12039103	20805	40	1402051
Caelo	Propifenazona	13332206	21454	60	20131009
Caelo	Propifenazona	23000810002	26747	40	20230526
Caelo	Propifenazona	23000810002	26747SI	20	20230526
Fagron	Propifenazona	16E02-B08-327928	23261	40	20160602
Fagron	Propifenazona	16H25-B01-334972	23922	40	20161227
Fagron	Propifenazona	20C20-B08-202174	25492	40	20200326

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Propifenazona*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Propifenazona*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propifenazona	15348908	23254	40
Caelo	Propifenazona	172776	23861	40
Caelo	Propifenazona	190190	24528	40
Fagron	Propifenazona	23G05-B08-229442	26904	40
Fagron	Propifenazona	23G05-B08-229442	26904SI	20

- 201 904 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 83 spectra from 34 *Apo-Ident* customers from 41 batches from the substance/substance group *Propifenazona*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Propifenazona	21000426007	1
Anzag	Propifenazona	19019003	1
Anzag	Propifenazona	21000426004	1
Caelo	Propifenazona	12039101	2
Caelo	Propifenazona	12039103	1
Caelo	Propifenazona	12039112	1
Caelo	Propifenazona	13036702	2
Caelo	Propifenazona	13137104	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propifenazona	13332205	3
Caelo	Propifenazona	15122502	1
Caelo	Propifenazona	15122504	3
Caelo	Propifenazona	15122505	1
Caelo	Propifenazona	15348901	2
Caelo	Propifenazona	15348902	2
Caelo	Propifenazona	15348904	2
Caelo	Propifenazona	15348908	2
Caelo	Propifenazona	15348910	1
Caelo	Propifenazona	15348912	2
Caelo	Propifenazona	15348913	6
Caelo	Propifenazona	15348914	2
Caelo	Propifenazona	17351302	1
Caelo	Propifenazona	17351304	4
Caelo	Propifenazona	17351305	1
Caelo	Propifenazona	190190003	4
Caelo	Propifenazona	19019003	4
Caesar & Loretz GmbH	Propifenazona	17351304	1
Caesar & Loretz GmbH	Propifenazona	21000426002	1
Caleo/Direkt	Propifenazona	19019003	1
Caleo/Noweda	Propifenazona	15348913	1
Euro OTC	Propifenazona		1
Fagron	Propifenazona	13B12-B02-297171	1
Fagron	Propifenazona	13K20-B03	2
Fagron	Propifenazona	13K20-B03-302291	1
Fagron	Propifenazona	13K20-B03-311715	3
Fagron	Propifenazona	13k20-b03-319137	1
Fagron	Propifenazona	13K20B03319137	1
Fagron	Propifenazona	13K20-B03-319137	3
Fagron	Propifenazona	13K-B03-319137	1
Fagron	Propifenazona	16E02-B08-327928	2
Fagron	Propifenazona	17G03-B01-347588	4
Fagron	Propifenazona	20A15-B04-196781	1
Fagron	Propifenazona	20C20-B08-202174	1
Fargon	Propifenazona	11H31-N07	1
Gatt-Koller / Phoenix	Propifenazona	419/02123112	1
Gatt-Koller	Propifenazona	1800011	1
Nachprüfung vom 31.0…	Propifenazona	13B12-B02-297171	1
Pharmachem	Propifenazona	15348913	1
Raben-Apotheke Mildenau	Propifenazona	12039103	1

- 235 984 spectra from 1515 *Apo-Ident* customers from a total of 49 217 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Propifenazona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propifenazona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	180	0	201 904
Type C	0	83	0	235 984

The substance/substance group *Propifenazona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.7711 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20805	20805	0,00	104,38
21454	20805	14,23	103,67
23261	20805	17,45	109,41
23922	20805	24,41	112,27
25492	20805	17,98	106,76
26747	20805	20,68	108,43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Propionato de clobetasol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20030-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propionato de clobetasol; Clobetasol, propionato; Clobetasoli propionas

Special notes

When selecting the *Propionato de clobetasol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Propionato de clobetasol	9	14	593

Second-stage model

For differentiation of the substance/substance group *Propionato de clobetasol* the following second-stage model is used:

- Submodelo 15

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Propionato de clobetasol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dipropionato de betametasona	52,73	61,97
⋮	⋮	⋮
Dipropionato de beclometasona	55,71	64,36

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Propionato de clobetasol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Propionato de clobetasol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propionato de clobetasol	13134705	21092	80	AR-15-FG-005328-01
Caelo	Propionato de clobetasol	13269505	21473	60	AR-15-FG-000622-02
Caelo	Propionato de clobetasol	14338001	21802	60	AR-16-FG-008581-01
Caelo	Propionato de clobetasol	14338001	21802SI	59	AR-16-FG-008581-01
Caelo	Propionato de clobetasol	14338001	21896	59	1607072
Caelo	Propionato de clobetasol	14338001	21896SI	45	1607072
Caelo	Propionato de clobetasol	15439504	22724	40	20160204
Caelo	Propionato de clobetasol	15439504	22724SI	37	20160204
Caelo	Propionato de clobetasol	192245	24904	40	20200127*
Euro OTC	Propionato de clobetasol	1211021-04	21611	60	1605044
Euro OTC	Propionato de clobetasol	1606022	22714	40	20160713*
Euro OTC	Propionato de clobetasol	1606022	22714SI	40	20160713*
Euro OTC	Propionato de clobetasol	2005025	25349	40	20200917*
Euro OTC	Propionato de clobetasol	2005025	25349SI	40	20200917*
Fagron	Propionato de clobetasol	18I12-B02-357669	24691	40	20181001

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 740 spectra of 15 reference samples from the substance/substance group *Propionato de clobetasol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 222 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1184 spectra of 30 reference samples from the substance/substance group *Propionato de clobetasol*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propionato de clobetasol	161067	22470	60
Caelo	Propionato de clobetasol	170967	23665	40
Caelo	Propionato de clobetasol	21001700	25793	40
Caelo	Propionato de clobetasol	24001314	27311	40
Euro OTC	Propionato de clobetasol	1704020	23397	40
Euro OTC	Propionato de clobetasol	1804002	24075	40
Euro OTC	Propionato de clobetasol	1903014	24615	40
Euro OTC	Propionato de clobetasol	2003026	25313	40
Euro OTC	Propionato de clobetasol	2109003	25870	50
Euro OTC	Propionato de clobetasol	2209014	26428	40
Euro OTC	Propionato de clobetasol	2406006	27346	40
Fagron	Propionato de clobetasol	19B06-B03-360421	24822	40
Fagron	Propionato de clobetasol	22L20-B03-227672	26546	40
Fagron	Propionato de clobetasol	23H24-B04-238756	27468	40
Caelo	Propionato de clobetasol	161067	22470SI	48
Caelo	Propionato de clobetasol	170967	23665SI	20
Caelo	Propionato de clobetasol	192245	24904SI†	40
Caelo	Propionato de clobetasol	21001700	25793SI	40
Caelo	Propionato de clobetasol	24001314	27311SI	34

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Propionato de clobetasol	1704020	23397SI	20
Euro OTC	Propionato de clobetasol	1804002	24075SI	22
Euro OTC	Propionato de clobetasol	1903014	24615SI	40
Euro OTC	Propionato de clobetasol	2003026	25313SI	40
Euro OTC	Propionato de clobetasol	2109003	25870SI	50
Euro OTC	Propionato de clobetasol	2209014	26428SI	40
Euro OTC	Propionato de clobetasol	2406006	27346SI	40
Fagron	Propionato de clobetasol	18I12-B02-357669	24691SI[†]	40
Fagron	Propionato de clobetasol	19B06-B03-360421	24822SI	40
Fagron	Propionato de clobetasol	22L20-B03-227672	26546SI	40
Fagron	Propionato de clobetasol	23H24-B04-238756	27468SI	40

- 200 900 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4444 spectra from 1179 *Apo-Ident* customers from 619 batches from the substance/substance group *Propionato de clobetasol*.

- Among them are spectra of independent samples from 592 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Propionato de clobetasol	11/29-N07	1
	Propionato de clobetasol	18044002-01	1
	Propionato de clobetasol	21001700015	1
	Propionato de clobetasol	21001700018	1
	Propionato de clobetasol	21001700021	3
	Propionato de clobetasol	21001700023	5
	Propionato de clobetasol	21001700025	6
	Propionato de clobetasol	21001700026	3
	Propionato de clobetasol	2100170025	1
	Propionato de clobetasol	2109003-001	1
	Propionato de clobetasol	2109003-01	11
	Propionato de clobetasol	21L16-B08-216942	1
	Propionato de clobetasol	21L16-B08-221088	1
	Propionato de clobetasol	21L16-B08	1
	Propionato de clobetasol	22090-01	1
	Propionato de clobetasol	2209014_01	1
	Propionato de clobetasol	2209014-01	16
	Propionato de clobetasol	2209014-02	2
	Propionato de clobetasol	22H25-B08-223089	1
	Propionato de clobetasol	22H-25-B08-223089	1
	Propionato de clobetasol	22H25-B08-223090	1
	Propionato de clobetasol	22H25-B08-225386	1
	Propionato de clobetasol	22L20-B03-227672	1
	Propionato de clobetasol	23000426001	22

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Propionato de clobetasol	23000426002	5
	Propionato de clobetasol	23000426003	18
	Propionato de clobetasol	23000426006	2
	Propionato de clobetasol	230033150003	1
	Propionato de clobetasol	23003315001	2
	Propionato de clobetasol	23003315003	2
	Propionato de clobetasol	23D01-B01-228378	2
	Propionato de clobetasol	23G04-B08-232382	1
	Propionato de clobetasol	CL0001/0722	1
/Sanacorp	Propionato de clobetasol	1804002-01	3
170420-01	Propionato de clobetasol	17A057	1
20.12.2016 Phoenix 17,49EUR	Propionato de clobetasol	15439504	1
AHC	Propionato de clobetasol	1903014-01	5
AHC	Propionato de clobetasol	23D01-B01-227673	1
AHD 14.06.19 Ek: 18,50	Propionato de clobetasol	18082718	1
AHD	Propionato de clobetasol	17E04-B02-338441	1
AHD	Propionato de clobetasol	17L18-B02-347993	1
AHD	Propionato de clobetasol	18/12-B02-35302	1
AHD	Propionato de clobetasol	18/12-B02-355390	1
AHD	Propionato de clobetasol	18/12-B02-357669	1
AHD	Propionato de clobetasol	19j02-f02-3653202	1
AHD	Propionato de clobetasol	20F24-F03-374147	1
AHD	Propionato de clobetasol	21F11-B01	1
AHD	Propionato de clobetasol	21L16-B08-221088	1
AHD	Propionato de clobetasol	2209014-01	2
AHD	Propionato de clobetasol	F02-3653202	1
AHD	Propionato de clobetasol	F03-3741407	1
AHZ	Propionato de clobetasol	1606022	1
Alliance H.	Propionato de clobetasol	15234002	2
Alliance Health 17.0...	Propionato de clobetasol	APB00547/112010C	1
Alliance Healthcare	Propionato de clobetasol	12J25-N01	1
Alliance Healthcare	Propionato de clobetasol	18082714	1
Alliance Healthcare	Propionato de clobetasol	18I12-B02-357669	1
Alliance Healthcare	Propionato de clobetasol	1903014-01	3
Alliance Healthcare	Propionato de clobetasol	21001700003	1
Alliance Healthcare	Propionato de clobetasol	21001700007	1
Alliance Healthcare	Propionato de clobetasol	21L16-B08-221090	1
Alliance	Propionato de clobetasol	12342305	1
Alliance	Propionato de clobetasol	21001700023	1
Allianz Healthcare 0...	Propionato de clobetasol	1408018-01	1
Allianz Healthcare	Propionato de clobetasol	18082709	1
allianz	Propionato de clobetasol	15234009	1
Allianz	Propionato de clobetasol	17325606	1
Anzag	Propionato de clobetasol	1211021-02	1
Anzag	Propionato de clobetasol	12E08-N04	1
Anzag	Propionato de clobetasol	1408018-01	2
Anzag	Propionato de clobetasol	15246001	1
Anzag	Propionato de clobetasol	16106703	1
Anzag	Propionato de clobetasol	192245012	1
Anzag	Propionato de clobetasol	21001700003	1
Anzag	Propionato de clobetasol	2109003-01	1
Anzag	Propionato de clobetasol	CL0103/0220	1
apo-ident	Propionato de clobetasol	1606022-01	2
apomix	Propionato de clobetasol	1211021-03	1
apomix	Propionato de clobetasol	16106703	1
apomix	Propionato de clobetasol	16G18-B02-325571	1
apomix	Propionato de clobetasol	200502501	2
Audor Pharma	Propionato de clobetasol	ABCLP/M/036/16C	1
Audor Pharma	Propionato de clobetasol	APAPL/035/E-12C	2
Audor Pharma	Propionato de clobetasol	APB0054/112010C	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Propionato de clobetasol	APCLO102/0518C	8
Audor Pharma	Propionato de clobetasol	APCLP	1
Audor Pharma	Propionato de clobetasol	APCLP/M/036/16C	5
Audor Pharma	Propionato de clobetasol	APL/035/E-12C	1
Audor Pharma	Propionato de clobetasol	APL035E12C	1
Audor Pharma	Propionato de clobetasol	sieheBemerkung	1
Bombastus	Propionato de clobetasol	12342303	1
Bombastus	Propionato de clobetasol	13G23-NO	1
Bombastus	Propionato de clobetasol	13G23-NO1	1
Bombastus	Propionato de clobetasol	1804002-01	2
Caelo	Propionato de clobetasol		1
Caelo	Propionato de clobetasol	1070317/16106704	1
Caelo	Propionato de clobetasol	1105044-03	1
Caelo	Propionato de clobetasol	1108044-02	1
Caelo	Propionato de clobetasol	1108044-03	2
Caelo	Propionato de clobetasol	1108044-04	1
Caelo	Propionato de clobetasol	1110116	1
Caelo	Propionato de clobetasol	11101311	1
Caelo	Propionato de clobetasol	11101315	1
Caelo	Propionato de clobetasol	11300702	3
Caelo	Propionato de clobetasol	11300703	5
Caelo	Propionato de clobetasol	11300707	2
Caelo	Propionato de clobetasol	12107601	3
Caelo	Propionato de clobetasol	12107602	3
Caelo	Propionato de clobetasol	12107604	1
Caelo	Propionato de clobetasol	12107606	1
Caelo	Propionato de clobetasol	12107607	6
Caelo	Propionato de clobetasol	12107608	1
Caelo	Propionato de clobetasol	12107609	6
Caelo	Propionato de clobetasol	121102104	1
Caelo	Propionato de clobetasol	12342303	1
Caelo	Propionato de clobetasol	12342306	6
Caelo	Propionato de clobetasol	12342307	3
Caelo	Propionato de clobetasol	12342308	1
Caelo	Propionato de clobetasol	12342309	14
Caelo	Propionato de clobetasol	12342310	7
Caelo	Propionato de clobetasol	12342312	1
Caelo	Propionato de clobetasol	123645	1
Caelo	Propionato de clobetasol	12E08-N04	1
Caelo	Propionato de clobetasol	12J25-N01	1
Caelo	Propionato de clobetasol	13134701	17
Caelo	Propionato de clobetasol	13134702	7
Caelo	Propionato de clobetasol	13134703	4
Caelo	Propionato de clobetasol	13134704	4
Caelo	Propionato de clobetasol	13134705	4
Caelo	Propionato de clobetasol	13269501	1
Caelo	Propionato de clobetasol	13269502	3
Caelo	Propionato de clobetasol	13269504	6
Caelo	Propionato de clobetasol	13269505	2
Caelo	Propionato de clobetasol	13269506	1
Caelo	Propionato de clobetasol	13269507	3
Caelo	Propionato de clobetasol	13269508	13
Caelo	Propionato de clobetasol	13269509	1
Caelo	Propionato de clobetasol	13269510	2
Caelo	Propionato de clobetasol	1369504	1
Caelo	Propionato de clobetasol	13A02-N04	1
Caelo	Propionato de clobetasol	13G23-N01	1
Caelo	Propionato de clobetasol	13K08-B30-287726	1
Caelo	Propionato de clobetasol	13K08-B30-287728	1
Caelo	Propionato de clobetasol	1408018-02	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propionato de clobetasol	1408018-03	10
Caelo	Propionato de clobetasol	14102416	1
Caelo	Propionato de clobetasol	14188501	4
Caelo	Propionato de clobetasol	14188502	8
Caelo	Propionato de clobetasol	14188503	17
Caelo	Propionato de clobetasol	14188504	7
Caelo	Propionato de clobetasol	14188506	3
Caelo	Propionato de clobetasol	14338001	9
Caelo	Propionato de clobetasol	14338002	3
Caelo	Propionato de clobetasol	14338005	3
Caelo	Propionato de clobetasol	14338006	11
Caelo	Propionato de clobetasol	14338007	6
Caelo	Propionato de clobetasol	14338008	5
Caelo	Propionato de clobetasol	1438007	1
Caelo	Propionato de clobetasol	14C03-B07-293560	2
Caelo	Propionato de clobetasol	14G30_B07_302114	1
Caelo	Propionato de clobetasol	14G30-B07-302114	2
Caelo	Propionato de clobetasol	14g30bo7302114	1
Caelo	Propionato de clobetasol	15031401	1
Caelo	Propionato de clobetasol	152340004	1
Caelo	Propionato de clobetasol	15234001	11
Caelo	Propionato de clobetasol	15234002	1
Caelo	Propionato de clobetasol	15234003	19
Caelo	Propionato de clobetasol	15234004	22
Caelo	Propionato de clobetasol	15234008	1
Caelo	Propionato de clobetasol	15234009	7
Caelo	Propionato de clobetasol	1524003	1
Caelo	Propionato de clobetasol	15246001	6
Caelo	Propionato de clobetasol	15253032	1
Caelo	Propionato de clobetasol	15412910	1
Caelo	Propionato de clobetasol	154390504	1
Caelo	Propionato de clobetasol	15439501	6
Caelo	Propionato de clobetasol	15439502	8
Caelo	Propionato de clobetasol	15439503	23
Caelo	Propionato de clobetasol	15439504	27
Caelo	Propionato de clobetasol	15439507	2
Caelo	Propionato de clobetasol	1543953	1
Caelo	Propionato de clobetasol	15A14-B02	1
Caelo	Propionato de clobetasol	15C23-B02-310473	2
Caelo	Propionato de clobetasol	15J-15-B04-316616	1
Caelo	Propionato de clobetasol	15j15-b04-317698	1
Caelo	Propionato de clobetasol	160115CP	1
Caelo	Propionato de clobetasol	1606022	1
Caelo	Propionato de clobetasol	160602201	1
Caelo	Propionato de clobetasol	1606022-01	4
Caelo	Propionato de clobetasol	1606022-02	6
Caelo	Propionato de clobetasol	1606022-025349	1
Caelo	Propionato de clobetasol	160829CP	1
Caelo	Propionato de clobetasol	160919Di	1
Caelo	Propionato de clobetasol	1610670	1
Caelo	Propionato de clobetasol	16106701	5
Caelo	Propionato de clobetasol	16106702	16
Caelo	Propionato de clobetasol	16106703	22
Caelo	Propionato de clobetasol	16106704	28
Caelo	Propionato de clobetasol	16106709	21
Caelo	Propionato de clobetasol	16106710	12
Caelo	Propionato de clobetasol	16106711	26
Caelo	Propionato de clobetasol	16106712	5
Caelo	Propionato de clobetasol	16106713	6
Caelo	Propionato de clobetasol	16106715	9

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propionato de clobetasol	16106718	3
Caelo	Propionato de clobetasol	16106719	6
Caelo	Propionato de clobetasol	16106720	8
Caelo	Propionato de clobetasol	16107704	1
Caelo	Propionato de clobetasol	1616703	1
Caelo	Propionato de clobetasol	1616715	1
Caelo	Propionato de clobetasol	16348001	1
Caelo	Propionato de clobetasol	16353208	1
Caelo	Propionato de clobetasol	16C18-B02-325573	1
Caelo	Propionato de clobetasol	16E04-B12	1
Caelo	Propionato de clobetasol	16E04-B12-321034	4
Caelo	Propionato de clobetasol	16E04-B12-321036	1
Caelo	Propionato de clobetasol	16E04-B12-322020	2
Caelo	Propionato de clobetasol	16G18-B02-324627	1
Caelo	Propionato de clobetasol	16G18-B02-325572	1
Caelo	Propionato de clobetasol	16H22-B07-328012	1
Caelo	Propionato de clobetasol	1704020	1
Caelo	Propionato de clobetasol	170402001	2
Caelo	Propionato de clobetasol	1704020-01	17
Caelo	Propionato de clobetasol	170404CP1606022-02	1
Caelo	Propionato de clobetasol	17090708	1
Caelo	Propionato de clobetasol	17096701	13
Caelo	Propionato de clobetasol	17096702	9
Caelo	Propionato de clobetasol	17096703	2
Caelo	Propionato de clobetasol	17096704	5
Caelo	Propionato de clobetasol	17096705	23
Caelo	Propionato de clobetasol	17096706	24
Caelo	Propionato de clobetasol	17096706/1180418	1
Caelo	Propionato de clobetasol	17096707	16
Caelo	Propionato de clobetasol	17096708	38
Caelo	Propionato de clobetasol	17096709	12
Caelo	Propionato de clobetasol	1709704	1
Caelo	Propionato de clobetasol	17097608	1
Caelo	Propionato de clobetasol	17325601	15
Caelo	Propionato de clobetasol	17325602	39
Caelo	Propionato de clobetasol	17325603	22
Ĉaelo	Propionato de clobetasol	17325604	1
Caelo	Propionato de clobetasol	17325605	20
Caelo	Propionato de clobetasol	17325606	4
Caelo	Propionato de clobetasol	17325607	1
Caelo	Propionato de clobetasol	1735603	1
Caelo	Propionato de clobetasol	17E04-B02-336882	1
Caelo	Propionato de clobetasol	17g14	1
Caelo	Propionato de clobetasol	17G14-B12-340176	1
Caelo	Propionato de clobetasol	17G14-B12-341742	1
Caelo	Propionato de clobetasol	17L18-B02-347993	1
Caelo	Propionato de clobetasol	18/12-B02-353203	1
Caelo	Propionato de clobetasol	18/12-B02-35480	1
Caelo	Propionato de clobetasol	18/12-B02-355390	1
Caelo	Propionato de clobetasol	18/12-b02-355657	1
Caelo	Propionato de clobetasol	180400201	2
Caelo	Propionato de clobetasol	1804002-01	14
Caelo	Propionato de clobetasol	18040020108638392	1
Caelo	Propionato de clobetasol	18082701	1
Caelo	Propionato de clobetasol	18082702	14
Caelo	Propionato de clobetasol	18082703	29
Caelo	Propionato de clobetasol	18082708	27
Caelo	Propionato de clobetasol	18082709	36
Caelo	Propionato de clobetasol	18082710	21
Caelo	Propionato de clobetasol	18082711	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propionato de clobetasol	18082714	14
Caelo	Propionato de clobetasol	18082717	6
Caelo	Propionato de clobetasol	18082718	14
Caelo	Propionato de clobetasol	180827708	1
Caelo	Propionato de clobetasol	181016709	1
Caelo	Propionato de clobetasol	1812B02355390	1
Caelo	Propionato de clobetasol	183000204	2
Caelo	Propionato de clobetasol	183000209	1
Caelo	Propionato de clobetasol	183002001	5
Caelo	Propionato de clobetasol	18300202	6
Caelo	Propionato de clobetasol	18300203	18
Caelo	Propionato de clobetasol	18300204	20
Caelo	Propionato de clobetasol	18300204P-191206-1	1
Caelo	Propionato de clobetasol	18300207	2
Caelo	Propionato de clobetasol	18300208	20
Caelo	Propionato de clobetasol	18300209	24
Caelo	Propionato de clobetasol	18300210	27
Caelo	Propionato de clobetasol	18300212	11
Caelo	Propionato de clobetasol	18300213	18
Caelo	Propionato de clobetasol	1830024	1
Caelo	Propionato de clobetasol	18H22-B017-328012	1
Caelo	Propionato de clobetasol	190301401	1
Caelo	Propionato de clobetasol	1922245002	1
Caelo	Propionato de clobetasol	192245002	19
Caelo	Propionato de clobetasol	192245003	24
Caelo	Propionato de clobetasol	192245004	25
Caelo	Propionato de clobetasol	192245007	12
Caelo	Propionato de clobetasol	192245009	16
Caelo	Propionato de clobetasol	192245011	43
Caelo	Propionato de clobetasol	192245012	18
Caelo	Propionato de clobetasol	192245012/5020	1
Caelo	Propionato de clobetasol	192245014	1
Caelo	Propionato de clobetasol	192245015	14
Caelo	Propionato de clobetasol	19224507	1
Caelo	Propionato de clobetasol	19224514	1
Caelo	Propionato de clobetasol	1922455004	1
Caelo	Propionato de clobetasol	19300213	1
Caelo	Propionato de clobetasol	19G23-B05-363805	1
Caelo	Propionato de clobetasol	20004302002	17
Caelo	Propionato de clobetasol	20004302003	49
Caelo	Propionato de clobetasol	20004302004	1
Caelo	Propionato de clobetasol	20004302006	11
Caelo	Propionato de clobetasol	20004302009	18
Caelo	Propionato de clobetasol	200043202009	1
Caelo	Propionato de clobetasol	20043202003	1
Caelo	Propionato de clobetasol	2005025-01	5
Caelo	Propionato de clobetasol	20111700001	1
Caelo	Propionato de clobetasol	20121012-4	1
Caelo	Propionato de clobetasol	2014E-02835	1
Caelo	Propionato de clobetasol	20F24-F03-374147	2
Caelo	Propionato de clobetasol	21001700001	21
Caelo	Propionato de clobetasol	21001700003	30
Caelo	Propionato de clobetasol	21001700004	2
Caelo	Propionato de clobetasol	21001700007	31
Caelo	Propionato de clobetasol	21001700008	27
Caelo	Propionato de clobetasol	2100170001	2
Caelo	Propionato de clobetasol	21001700011	2
Caelo	Propionato de clobetasol	21001700013	38
Caelo	Propionato de clobetasol	21001700015	13
Caelo	Propionato de clobetasol	21001700018	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propionato de clobetasol	21001700019	1
Caelo	Propionato de clobetasol	21001700021	11
Caelo	Propionato de clobetasol	21001700023	1
Caelo	Propionato de clobetasol	21001700025	3
Caelo	Propionato de clobetasol	21001700026	7
Caelo	Propionato de clobetasol	21001700027	2
Caelo	Propionato de clobetasol	2100170003	3
Caelo	Propionato de clobetasol	2100170013	1
Caelo	Propionato de clobetasol	2100170015	1
Caelo	Propionato de clobetasol	2100170026	1
Caelo	Propionato de clobetasol	210170015	1
Caelo	Propionato de clobetasol	23000426006	6
Caelo	Propionato de clobetasol	23111202	1
Caelo	Propionato de clobetasol	2778	1
Caelo	Propionato de clobetasol	2829	1
Caelo	Propionato de clobetasol	2x17325602	1
Caelo	Propionato de clobetasol	3012Q02835	1
Caelo	Propionato de clobetasol	31071302	1
Caelo	Propionato de clobetasol	3110350	1
Caelo	Propionato de clobetasol	3440	1
Caelo	Propionato de clobetasol	36/AKD2	1
Caelo	Propionato de clobetasol	4/0216	1
Caelo	Propionato de clobetasol	5119U02835	1
Caelo	Propionato de clobetasol	8082703	1
Caelo	Propionato de clobetasol	apl/294/b-14	1
Caelo	Propionato de clobetasol	CLO/1191217	1
Caelo	Propionato de clobetasol	CLO004/0216	1
Caelo	Propionato de clobetasol	CLO024/0915	1
Caeolo /Sana	Propionato de clobetasol	18082711	1
Caeolo/Krieger	Propionato de clobetasol	17096706	3
Caeolo/Noweda	Propionato de clobetasol	15439503	1
Caeolo	Propionato de clobetasol	17096709	1
Caesar & Loretz /Phönix	Propionato de clobetasol	20004302003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300212	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300210	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245009	2
Caesar & Loretz GmbH...	Propionato de clobetasol	18300204	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300213	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18082718	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245002	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245011	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18082709	2
Caesar & Loretz GmbH...	Propionato de clobetasol	192245002	2
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302009	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700007	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245002	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245011	2
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700021	1
Caesar & Loretz GmbH/AEP	Propionato de clobetasol	18300203	1
Caesar & Loretz GmbH/AHD	Propionato de clobetasol	20004302009	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18082714	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300204	1
Caesar & Loretz GmbH/G	Propionato de clobetasol	20004302003	1
Caesar & Loretz GmbH/Gehe	Propionato de clobetasol	18082702	1
Caesar & Loretz GmbH/Gehe	Propionato de clobetasol	18082714	1
Caesar & Loretz GmbH/Gehe	Propionato de clobetasol	192245002	1
Caesar & Loretz GmbH/Gehe	Propionato de clobetasol	192245004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Propionato de clobetasol	20004302002	2
Caesar & Loretz GmbH/Gehe	Propionato de clobetasol	21001700008	1
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302004	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700013	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300213	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245002	1
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	23000426001	1
Caesar & Loretz GmbH...	Propionato de clobetasol	AP221112-02	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300212	2
Caesar & Loretz GmbH/l10	Propionato de clobetasol	21001700013	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245004	2
Caesar & Loretz GmbH...	Propionato de clobetasol	192245009	1
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302009	2
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700001	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700008	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700015	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700021	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300213	1
Caesar & Loretz GmbH...	Propionato de clobetasol	20004302009	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300204	2
Caesar & Loretz GmbH...	Propionato de clobetasol	18300212	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245007	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700007	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700013	1
Caesar & Loretz GmbH/Sana	Propionato de clobetasol	21001700003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18082709	1
Caesar & Loretz GmbH...	Propionato de clobetasol	18300212	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245003	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245007	1
Caesar & Loretz GmbH...	Propionato de clobetasol	192245011	1
Caesar & Loretz GmbH...	Propionato de clobetasol	21001700013	2
Caesar & Loretz GmbH	Propionato de clobetasol	16106702	3
Caesar & Loretz GmbH	Propionato de clobetasol	18082703	1
Caesar & Loretz GmbH	Propionato de clobetasol	18082708	4
Caesar & Loretz GmbH	Propionato de clobetasol	18082709	8
Caesar & Loretz GmbH	Propionato de clobetasol	18082710	4
Caesar & Loretz GmbH	Propionato de clobetasol	18082711	1
Caesar & Loretz GmbH	Propionato de clobetasol	18082714	4
Caesar & Loretz GmbH	Propionato de clobetasol	18082718	6
Caesar & Loretz GmbH	Propionato de clobetasol	183002001	3
Caesar & Loretz GmbH	Propionato de clobetasol	18300202	2
Caesar & Loretz GmbH	Propionato de clobetasol	18300203	2
Caesar & Loretz GmbH	Propionato de clobetasol	18300204	12
Caesar & Loretz GmbH	Propionato de clobetasol	18300208	8
Caesar & Loretz GmbH	Propionato de clobetasol	18300209	9
Caesar & Loretz GmbH	Propionato de clobetasol	18300210	5
Caesar & Loretz GmbH	Propionato de clobetasol	18300212	5
Caesar & Loretz GmbH	Propionato de clobetasol	18300213	6
Caesar & Loretz GmbH	Propionato de clobetasol	192245002	10
Caesar & Loretz GmbH	Propionato de clobetasol	192245003	10
Caesar & Loretz GmbH	Propionato de clobetasol	192245004	5
Caesar & Loretz GmbH	Propionato de clobetasol	192245005	1
Caesar & Loretz GmbH	Propionato de clobetasol	192245007	7
Caesar & Loretz GmbH	Propionato de clobetasol	192245009	5
Caesar & Loretz GmbH	Propionato de clobetasol	192245011	19
Caesar & Loretz GmbH	Propionato de clobetasol	192245012	4
Caesar & Loretz GmbH	Propionato de clobetasol	192245015	2
Caesar & Loretz GmbH	Propionato de clobetasol	20004302002	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Propionato de clobetasol	20004302003	23
Caesar & Loretz GmbH	Propionato de clobetasol	20004302006	4
Caesar & Loretz GmbH	Propionato de clobetasol	20004302009	6
Caesar & Loretz GmbH	Propionato de clobetasol	21001700001	6
Caesar & Loretz GmbH	Propionato de clobetasol	21001700002	1
Caesar & Loretz GmbH	Propionato de clobetasol	21001700003	9
Caesar & Loretz GmbH	Propionato de clobetasol	21001700004	2
Caesar & Loretz GmbH	Propionato de clobetasol	21001700007	4
Caesar & Loretz GmbH	Propionato de clobetasol	21001700008	3
Caesar & Loretz GmbH	Propionato de clobetasol	21001700011	2
Caesar & Loretz GmbH	Propionato de clobetasol	21001700013	9
Caesar & Loretz GmbH	Propionato de clobetasol	21001700015	5
Caesar & Loretz GmbH	Propionato de clobetasol	21001700019	1
Caesar & Loretz GmbH	Propionato de clobetasol	21001700021	3
Caesar & Loretz GmbH	Propionato de clobetasol	21001700025	4
Caesar & Loretz GmbH	Propionato de clobetasol	F02-3669403	1
Caesar & Loretz Hild...	Propionato de clobetasol	192245002	1
Caesar & Loretz Hild...	Propionato de clobetasol	192245003	1
Caesar & Loretz Hild...	Propionato de clobetasol	192245011	1
Caesar & Loretz Hilden	Propionato de clobetasol	18300204	1
Caesar & Loretz Hilden	Propionato de clobetasol	18300213	1
Caesar & Loretz/ Noweda	Propionato de clobetasol	12342306	1
Caesar & Loretz/AHD	Propionato de clobetasol	192245003	1
Caesar & Loretz/Gehe	Propionato de clobetasol	192245011	1
Caesar & Loretz/Geil...	Propionato de clobetasol	20004302003	1
Caesar & Loretz/Noweda	Propionato de clobetasol	20004302009	1
Caesar & Loretz	Propionato de clobetasol	17096705	2
Caesar & Loretz	Propionato de clobetasol	192245015	1
Caesar & Loretz	Propionato de clobetasol	20004302002	1
Caesar Loretz	Propionato de clobetasol	192245011	1
Caesar u Loretz	Propionato de clobetasol	12107608	2
Caesar und Loretz	Propionato de clobetasol	18300203	1
Caesar und Loretz	Propionato de clobetasol	18300208	2
Caesar&Lorenz	Propionato de clobetasol	1610370	1
Caesar&Lorenz	Propionato de clobetasol	20004302002	1
Caesar&Loretz GmbH	Propionato de clobetasol	15234001	1
Caesar&Loretz GmbH	Propionato de clobetasol	15439501	1
Caesar&Loretz GmbH	Propionato de clobetasol	192245015	1
Caesar/Lorenz	Propionato de clobetasol	12342305	3
Caesar/Lorenz	Propionato de clobetasol	12342309	1
Caesar/Loretz	Propionato de clobetasol	12342310	1
Cealo /Gehe	Propionato de clobetasol	18082710	1
Cealo	Propionato de clobetasol	1408018	1
Cealo	Propionato de clobetasol	16106702	2
cealo	Propionato de clobetasol	16106703	1
Cealo	Propionato de clobetasol	192245003	1
Cealo	Propionato de clobetasol	21001700003	1
Chiesi/ Now	Propionato de clobetasol	13269503	3
Crystal Pharma	Propionato de clobetasol	C0054/1	1
Delta	Propionato de clobetasol	17096701	1
DR.WOLFF	Propionato de clobetasol	15J15-B04-317699	1
E Plus	Propionato de clobetasol	16106702	1
eur	Propionato de clobetasol	1704020-01	2
EuRho / Gehe	Propionato de clobetasol	1903014-01	4
EuRho / Noweda	Propionato de clobetasol	2109003-01	1
EuRho 06.10.2011 Anzag	Propionato de clobetasol	1108044-01	1
EuRho- Phoenix	Propionato de clobetasol	2109003-01	1
EuRho/ Anzag	Propionato de clobetasol	29(1903014-01)	1
EuRho/ NOWEDA	Propionato de clobetasol	1704020-01	1
EuRho/ NOWEDA	Propionato de clobetasol	1804002-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/ Phönix	Propionato de clobetasol	1704020-01	1
EuRho/Fiebig	Propionato de clobetasol	2005025-01	1
EuRho/Gehe	Propionato de clobetasol	1704020-01	2
EuRho/Noveda	Propionato de clobetasol	1804002-01	1
EuRho/Phoenix	Propionato de clobetasol	160602202	1
EuRho/Phoenix	Propionato de clobetasol	1903014	1
EuRho/Sanacorp	Propionato de clobetasol	1704020-01	1
EuRho/Sanacorp	Propionato de clobetasol	1903014-01	1
EuRho/Sanacorp	Propionato de clobetasol	2005025-01	1
EuRho/Sanacorp	Propionato de clobetasol	2109003-01	2
EuRho	Propionato de clobetasol	1108044-04	2
EuRho	Propionato de clobetasol	1408018-01	1
EuRho	Propionato de clobetasol	1408018-02	2
EuRho	Propionato de clobetasol	1704020-01	1
EuRho	Propionato de clobetasol	1804002-01	2
EuRho	Propionato de clobetasol	1903014-01	4
EuRho	Propionato de clobetasol	2109003-01	1
euro AHD	Propionato de clobetasol	1704020-015592	1
euro AHD	Propionato de clobetasol	1804002-015788	1
Euro OCT / Krieger	Propionato de clobetasol	1903014-01	1
Euro OT	Propionato de clobetasol	14081018-02	1
Euro OTC	Propionato de clobetasol	100402-01	1
Euro OTC	Propionato de clobetasol	1072015D	1
Euro OTC	Propionato de clobetasol	1105044-04	1
Euro OTC	Propionato de clobetasol	1108044	1
Euro OTC	Propionato de clobetasol	1108044-01	4
Euro OTC	Propionato de clobetasol	1108044-02	8
Euro OTC	Propionato de clobetasol	1108044-03	14
Euro OTC	Propionato de clobetasol	1108044-037-16	1
Euro OTC	Propionato de clobetasol	110804404	2
Euro OTC	Propionato de clobetasol	1108044-04	15
Euro OTC	Propionato de clobetasol	112/1018	1
Euro OTC	Propionato de clobetasol	1204037-01	1
Euro OTC	Propionato de clobetasol	12082013B	1
Euro OTC	Propionato de clobetasol	12110-01	1
Euro OTC	Propionato de clobetasol	1211021/02	1
Euro OTC	Propionato de clobetasol	121102101	2
Euro OTC	Propionato de clobetasol	1211021-01	20
Euro OTC	Propionato de clobetasol	1211021-02	31
Euro OTC	Propionato de clobetasol	1211021-03	30
Euro OTC	Propionato de clobetasol	1211021-04	21
Euro OTC	Propionato de clobetasol	121K021-01	1
Euro OTC	Propionato de clobetasol	13042015A	1
Euro OTC	Propionato de clobetasol	130604002	1
Euro OTC	Propionato de clobetasol	13G23-N01	1
Euro OTC	Propionato de clobetasol	1402018-03	1
Euro OTC	Propionato de clobetasol	14080-02	1
Euro OTC	Propionato de clobetasol	1408015-01	1
Euro OTC	Propionato de clobetasol	1408018	1
Euro OTC	Propionato de clobetasol	140801801	1
Euro OTC	Propionato de clobetasol	1408018-01	17
Euro OTC	Propionato de clobetasol	140801802	1
Euro OTC	Propionato de clobetasol	1408018-02	78
Euro OTC	Propionato de clobetasol	140801803	2
Euro OTC	Propionato de clobetasol	1408018-03	32
Euro OTC	Propionato de clobetasol	140808-02	1
Euro OTC	Propionato de clobetasol	14080818-02	1
Euro OTC	Propionato de clobetasol	15234003	1
Euro OTC	Propionato de clobetasol	1601046-01	1
Euro OTC	Propionato de clobetasol	16042014C	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Propionato de clobetasol	1606022	3
Euro OTC	Propionato de clobetasol	160602201	6
Euro OTC	Propionato de clobetasol	1606022-01	32
Euro OTC	Propionato de clobetasol	160602202	6
Euro OTC	Propionato de clobetasol	1606022-02	62
Euro OTC	Propionato de clobetasol	160622-02	1
Euro OTC	Propionato de clobetasol	16106720	1
Euro OTC	Propionato de clobetasol	1704020	2
Euro OTC	Propionato de clobetasol	170402001	9
Euro OTC	Propionato de clobetasol	1704020-01	142
Euro OTC	Propionato de clobetasol	1704020-015498	1
Euro OTC	Propionato de clobetasol	17044020-01	2
Euro OTC	Propionato de clobetasol	17096705	1
Euro OTC	Propionato de clobetasol	17096709	1
Euro OTC	Propionato de clobetasol	171107CP/1704020-01	1
Euro OTC	Propionato de clobetasol	17E04-B02-338441	1
Euro OTC	Propionato de clobetasol	17L18-B02-347993	1
Euro OTC	Propionato de clobetasol	18004002-01	1
Euro OTC	Propionato de clobetasol	1801002-01	1
Euro OTC	Propionato de clobetasol	180400002	1
Euro OTC	Propionato de clobetasol	180400-01	1
Euro OTC	Propionato de clobetasol	18040002-01	1
Euro OTC	Propionato de clobetasol	1804001-01	1
Euro OTC	Propionato de clobetasol	1804002	1
Euro OTC	Propionato de clobetasol	180400201	5
Euro OTC	Propionato de clobetasol	1804002-01	191
Euro OTC	Propionato de clobetasol	1804002201	1
Euro OTC	Propionato de clobetasol	1804002-41	1
Euro OTC	Propionato de clobetasol	18041808	1
Euro OTC	Propionato de clobetasol	18082703	2
Euro OTC	Propionato de clobetasol	18082708	1
Euro OTC	Propionato de clobetasol	18082709	1
Euro OTC	Propionato de clobetasol	18082717	1
Euro OTC	Propionato de clobetasol	18111403	1
Euro OTC	Propionato de clobetasol	1903014	1
Euro OTC	Propionato de clobetasol	190301401	5
Euro OTC	Propionato de clobetasol	1903014-01	179
Euro OTC	Propionato de clobetasol	19030414-01	1
Euro OTC	Propionato de clobetasol	19031401	1
Euro OTC	Propionato de clobetasol	191142210	1
Euro OTC	Propionato de clobetasol	200025-01	1
Euro OTC	Propionato de clobetasol	2003023-01	1
Euro OTC	Propionato de clobetasol	2003026/01	2
Euro OTC	Propionato de clobetasol	200302601	1
Euro OTC	Propionato de clobetasol	2003026-01	10
Euro OTC	Propionato de clobetasol	200502501	11
Euro OTC	Propionato de clobetasol	2005025-01	121
Euro OTC	Propionato de clobetasol	200505-01	1
Euro OTC	Propionato de clobetasol	21001700008	2
Euro OTC	Propionato de clobetasol	21090003-01	1
Euro OTC	Propionato de clobetasol	210900301	4
Euro OTC	Propionato de clobetasol	2109003-01	76
Euro OTC	Propionato de clobetasol	2111I-02835	1
Euro OTC	Propionato de clobetasol	220826(2005025-01)	1
Euro OTC	Propionato de clobetasol	2209014-01	1
Euro OTC	Propionato de clobetasol	2835	1
Euro OTC	Propionato de clobetasol	30092014A	1
Euro OTC	Propionato de clobetasol	31606022-02	1
Euro OTC	Propionato de clobetasol	4091512	1
Euro OTC	Propionato de clobetasol	4113Q-02835	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Propionato de clobetasol	700225	2
Euro OTC	Propionato de clobetasol	80616-1	1
Euro OTC	Propionato de clobetasol	819081-39	1
Euro OTC	Propionato de clobetasol	CLO105-0519	1
Euro OTC	Propionato de clobetasol	CLO112/1018	2
Euro OTC	Propionato de clobetasol	CLO119/1217	2
Euro OTC	Propionato de clobetasol	Clob100123	1
Euro OTC	Propionato de clobetasol	CLO-BL2153/0711	1
Euro OTC	Propionato de clobetasol	CLO-BL2322/1012	2
Euro OTC	Propionato de clobetasol	CLO-BLT223/1216	1
Euro OTC	Propionato de clobetasol	clo-blt223/126	1
Euro OTC	Propionato de clobetasol	EuroOTC	4
Euro OTC	Propionato de clobetasol	P14091725/1606022-01	1
Euro/ANZAG	Propionato de clobetasol	1606022-02	1
Euro/ANZAG	Propionato de clobetasol	1804002-01	1
EuRo/Anzag	Propionato de clobetasol	1804002-01	3
Euro/ANZAG	Propionato de clobetasol	1903014-01	1
Euro/Phönix	Propionato de clobetasol	210900301	1
euro/Symbiotica/Alli	Propionato de clobetasol	1903014-01	1
Euro	Propionato de clobetasol	1211021-02	2
EuRoh/ Gehe	Propionato de clobetasol	1804002-01	2
euroho/gehe	Propionato de clobetasol	1211021-01	1
EurRho/Noweda	Propionato de clobetasol	2005025-01	1
Eurro/Phoenix	Propionato de clobetasol	1804002-01	1
Fagon / Gehe	Propionato de clobetasol	18/12-B02-354809	1
Fagron	Propionato de clobetasol		1
Fagron	Propionato de clobetasol	11/29-N07	1
Fagron	Propionato de clobetasol	11-05-N06	1
Fagron	Propionato de clobetasol	11300703	1
Fagron	Propionato de clobetasol	11C16-NO1	1
Fagron	Propionato de clobetasol	11D26-N04	1
Fagron	Propionato de clobetasol	11H10-N02	1
Fagron	Propionato de clobetasol	11L12-N05	2
Fagron	Propionato de clobetasol	11129-N07	1
Fagron	Propionato de clobetasol	1211021	1
Fagron	Propionato de clobetasol	1211021-02	1
Fagron	Propionato de clobetasol	12A02-N04	1
Fagron	Propionato de clobetasol	12E08N04	1
Fagron	Propionato de clobetasol	12E08-N04	11
Fagron	Propionato de clobetasol	12J25-N01	5
Fagron	Propionato de clobetasol	1314705	1
Fagron	Propionato de clobetasol	13A02-N04	18
Fagron	Propionato de clobetasol	13Ao2-N04	1
Fagron	Propionato de clobetasol	13G23N01	1
Fagron	Propionato de clobetasol	13G23-N01	18
Fagron	Propionato de clobetasol	13G23-N01NT0421M	1
Fagron	Propionato de clobetasol	13G23-NO1	1
Fagron	Propionato de clobetasol	13K08-B03-287728	1
Fagron	Propionato de clobetasol	13K08-B30	2
Fagron	Propionato de clobetasol	13K08-B30-287726	2
Fagron	Propionato de clobetasol	13K08B30287727	1
Fagron	Propionato de clobetasol	13K08-B30-287727	2
Fagron	Propionato de clobetasol	13-K08-B30-287727	1
Fagron	Propionato de clobetasol	13k08b30287728	1
Fagron	Propionato de clobetasol	13K08-B30-287728	6
Fagron	Propionato de clobetasol	13K08-B30-287729	2
Fagron	Propionato de clobetasol	13K08B30287730	1
Fagron	Propionato de clobetasol	13K08-B30-287730	2
Fagron	Propionato de clobetasol	1405018-02	1
Fagron	Propionato de clobetasol	14C03-B07	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propionato de clobetasol	14C03-B07-293560	1
Fagron	Propionato de clobetasol	14C03-B07-293561	2
Fagron	Propionato de clobetasol	14C03-B07-293562	9
Fagron	Propionato de clobetasol	14C03-B07-293563	2
Fagron	Propionato de clobetasol	14C03-B07-305985	1
Fagron	Propionato de clobetasol	14C03-B07-305986	2
Fagron	Propionato de clobetasol	14C03-B07-305987	2
Fagron	Propionato de clobetasol	14G30_B07_302112	1
Fagron	Propionato de clobetasol	14G30-B07	1
Fagron	Propionato de clobetasol	14G30-B07-302112	2
Fagron	Propionato de clobetasol	14G30-B07-302113	2
Fagron	Propionato de clobetasol	14G30-B07-302114	11
Fagron	Propionato de clobetasol	14G30-B07-302115	2
Fagron	Propionato de clobetasol	14G30B07-302116	1
Fagron	Propionato de clobetasol	14G30-B07-302116	4
Fagron	Propionato de clobetasol	14G30-B07-303114	1
Fagron	Propionato de clobetasol	15/15-B04-317699	1
Fagron	Propionato de clobetasol	15a14-b02-303125	2
Fagron	Propionato de clobetasol	15A14-B02-303125	12
Fagron	Propionato de clobetasol	15C23-B02_310473	2
Fagron	Propionato de clobetasol	15c23-b02-310473	2
Fagron	Propionato de clobetasol	15C23-B02-310473	12
Fagron	Propionato de clobetasol	15C23-B02-310522	3
Fagron	Propionato de clobetasol	15G01-B02-311578	1
Fagron	Propionato de clobetasol	15H26-B03-312355	4
Fagron	Propionato de clobetasol	15H26-B03-312860	1
Fagron	Propionato de clobetasol	15J15-B04	1
Fagron	Propionato de clobetasol	15J15-B04-316615	1
Fagron	Propionato de clobetasol	15j15-B04-317698	1
Fagron	Propionato de clobetasol	15J15-B04-317698	6
Fagron	Propionato de clobetasol	15J15-B04-317699	1
Fagron	Propionato de clobetasol	1606022-02	1
Fagron	Propionato de clobetasol	16106704	1
Fagron	Propionato de clobetasol	16E04-B12	1
Fagron	Propionato de clobetasol	16E04-B12-321032	1
Fagron	Propionato de clobetasol	16E04-B12-321033	3
Fagron	Propionato de clobetasol	16E04-B12-321034	3
Fagron	Propionato de clobetasol	16E04-B12-321035	1
Fagron	Propionato de clobetasol	16E04-B12-321036	2
Fagron	Propionato de clobetasol	16E04-B12-322020	4
Fagron	Propionato de clobetasol	16G18-B02-324627	6
Fagron	Propionato de clobetasol	16G18B02325571	1
Fagron	Propionato de clobetasol	16G18-B02-325571	2
Fagron	Propionato de clobetasol	16G18-B02-325572	1
Fagron	Propionato de clobetasol	16G18-B02-325573	8
Fagron	Propionato de clobetasol	16G18-B02-32571	1
Fagron	Propionato de clobetasol	16H22-B07	1
Fagron	Propionato de clobetasol	16H22-B07-328012	14
Fagron	Propionato de clobetasol	16H22-B07-330169	3
Fagron	Propionato de clobetasol	16K24-B04	2
Fagron	Propionato de clobetasol	16K24-B04-331220	1
Fagron	Propionato de clobetasol	16k24-b04-332086	1
Fagron	Propionato de clobetasol	16K24-B04-332086	6
Fagron	Propionato de clobetasol	16K24-B04-333120	6
Fagron	Propionato de clobetasol	16K24B04333121	1
Fagron	Propionato de clobetasol	16K24-B04-333121	3
Fagron	Propionato de clobetasol	16K24-B04-333143	5
Fagron	Propionato de clobetasol	16K24-B04-333120	1
Fagron	Propionato de clobetasol	170402001	1
Fagron	Propionato de clobetasol	1704020-01	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propionato de clobetasol	17096708	1
Fagron	Propionato de clobetasol	17E04B02335335	1
Fagron	Propionato de clobetasol	17E04-B02-335335	5
Fagron	Propionato de clobetasol	17E04B02336882	1
Fagron	Propionato de clobetasol	17E04-B02-336882	2
Fagron	Propionato de clobetasol	17e04-b02-338441	1
Fagron	Propionato de clobetasol	17E04-B02-338441	6
Fagron	Propionato de clobetasol	17G14-B12	1
Fagron	Propionato de clobetasol	17G14-B12-340175	6
Fagron	Propionato de clobetasol	17G14-B12-340176	3
Fagron	Propionato de clobetasol	17G14-B12-341742	1
Fagron	Propionato de clobetasol	17g14-b12-341743	1
Fagron	Propionato de clobetasol	17G14-B12-341743	3
Fagron	Propionato de clobetasol	17L18-B02	3
Fagron	Propionato de clobetasol	17L18B02-344841	1
Fagron	Propionato de clobetasol	17L18-B02-344841	3
Fagron	Propionato de clobetasol	17L18-B02-344842	3
Fagron	Propionato de clobetasol	17L18-B02-345403	7
Fagron	Propionato de clobetasol	17L18-B02-345404	4
Fagron	Propionato de clobetasol	17L18B02347991	1
Fagron	Propionato de clobetasol	17L18-B02347991	1
Fagron	Propionato de clobetasol	17L18-B02-347991	1
Fagron	Propionato de clobetasol	17L18-B02-347992	4
Fagron	Propionato de clobetasol	17l18-b02-347993	1
Fagron	Propionato de clobetasol	17L18-B02-347993	7
Fagron	Propionato de clobetasol	17L18-B02-351867	3
Fagron	Propionato de clobetasol	17LK18-B02-344841	1
Fagron	Propionato de clobetasol	18/12-B02_357669	1
Fagron	Propionato de clobetasol	18/12-b02-0002	1
Fagron	Propionato de clobetasol	18/12-B02-353201	5
Fagron	Propionato de clobetasol	18/12-B02-353202	8
Fagron	Propionato de clobetasol	18/12-B02-353203	1
Fagron	Propionato de clobetasol	18/12-B02-354809	2
Fagron	Propionato de clobetasol	18/12-B02-355065	1
Fagron	Propionato de clobetasol	18/12-B02-355390	3
Fagron	Propionato de clobetasol	18/12-B02-355657	3
Fagron	Propionato de clobetasol	18/12-B02-357670	1
Fagron	Propionato de clobetasol	18/12-BO2-353202	2
Fagron	Propionato de clobetasol	18/12-BO2-354809	1
Fagron	Propionato de clobetasol	1804002-01	1
Fagron	Propionato de clobetasol	18112-B02-357669	1
Fagron	Propionato de clobetasol	1812-B02-353202	1
Fagron	Propionato de clobetasol	1812-B02-353203	1
Fagron	Propionato de clobetasol	18I12-02	1
Fagron	Propionato de clobetasol	18I12-B02	5
Fagron	Propionato de clobetasol	18I12-B02_357670	1
Fagron	Propionato de clobetasol	18I12-B02-353202	4
Fagron	Propionato de clobetasol	18I12-B02-353203	3
Fagron	Propionato de clobetasol	18I12-B02-355065	1
Fagron	Propionato de clobetasol	18I12-B02-355390	4
Fagron	Propionato de clobetasol	18I12-B02-355391	4
Fagron	Propionato de clobetasol	18I12-B02-357669	3
Fagron	Propionato de clobetasol	18I12-B02-357670	1
Fagron	Propionato de clobetasol	18I12-BO2-355391	1
Fagron	Propionato de clobetasol	18l12-B02-353202	1
Fagron	Propionato de clobetasol	18l12-B02-353203	1
Fagron	Propionato de clobetasol	18l12-B02-354809	1
Fagron	Propionato de clobetasol	18l12-B02-355065	1
Fagron	Propionato de clobetasol	18l12-B02-355657	2
Fagron	Propionato de clobetasol	18l12-B02-357669	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propionato de clobetasol	18112-Bo2-353201	1
Fagron	Propionato de clobetasol	19/L10F02-366943	1
Fagron	Propionato de clobetasol	1903014-01	1
Fagron	Propionato de clobetasol	19B06-B03	2
Fagron	Propionato de clobetasol	19B06-B03-360420	1
Fagron	Propionato de clobetasol	19B06-B03-360421	4
Fagron	Propionato de clobetasol	19B06-B03-360426	1
Fagron	Propionato de clobetasol	19b06-b03-360603	1
Fagron	Propionato de clobetasol	19B06-B03-360603	1
Fagron	Propionato de clobetasol	19B06-B03-60603	1
Fagron	Propionato de clobetasol	19G23_B05_363805	1
Fagron	Propionato de clobetasol	19G23-B05	3
Fagron	Propionato de clobetasol	19G23-B05-363804	3
Fagron	Propionato de clobetasol	19G23-B05-363805	6
Fagron	Propionato de clobetasol	19G23-B05-363806	11
Fagron	Propionato de clobetasol	19G23-B05-363808	2
Fagron	Propionato de clobetasol	19G23-BO5-363806	1
Fagron	Propionato de clobetasol	19J02-F02	3
Fagron	Propionato de clobetasol	19J02-F02-365320	4
Fagron	Propionato de clobetasol	19J02-F02-365321	6
Fagron	Propionato de clobetasol	19J02F02-365322	1
Fagron	Propionato de clobetasol	19J02-F02365322	1
Fagron	Propionato de clobetasol	19J02-F02-365322	11
Fagron	Propionato de clobetasol	19J02-F02-365324	4
Fagron	Propionato de clobetasol	19JO2-F02-365322	1
Fagron	Propionato de clobetasol	19L10-F02	1
Fagron	Propionato de clobetasol	19L10-F02-3669402	1
Fagron	Propionato de clobetasol	19L10-F02-366941	6
Fagron	Propionato de clobetasol	19L10F02366942	1
Fagron	Propionato de clobetasol	19L10-F02-366942	7
Fagron	Propionato de clobetasol	19L10-F02-366942CLO113/0619	1
Fagron	Propionato de clobetasol	19L10F02366943	2
Fagron	Propionato de clobetasol	19L10-F02-366943	10
Fagron	Propionato de clobetasol	19L10-FO2-366945	1
Fagron	Propionato de clobetasol	20F24-F03-374147	8
Fagron	Propionato de clobetasol	20F24-F03-374148	3
Fagron	Propionato de clobetasol	20F-24-F03-374148	1
Fagron	Propionato de clobetasol	21F11-B01-213854	5
Fagron	Propionato de clobetasol	21f11-b01-217282	1
Fagron	Propionato de clobetasol	21F11-B01-217282	4
Fagron	Propionato de clobetasol	21L16-B08-216942	1
Fagron	Propionato de clobetasol	21L16-B08-218980	2
Fagron	Propionato de clobetasol	21L16-B08-221088	4
Fagron	Propionato de clobetasol	21L16-BO8-216879	1
Fagron	Propionato de clobetasol	21L6BO8	1
Fagron	Propionato de clobetasol	22H25B08	1
Fagron	Propionato de clobetasol	22L2O-B03-227672	1
Fagron	Propionato de clobetasol	341743	1
Fagron	Propionato de clobetasol	3713M-02835	1
Fagron	Propionato de clobetasol	B05-3638004	1
Fagron	Propionato de clobetasol	B05-3638006	1
Fagron	Propionato de clobetasol	B05-3680006	1
Fagron	Propionato de clobetasol	CLO001/0421	1
Fagron	Propionato de clobetasol	CLO002/0621	2
Fagron	Propionato de clobetasol	CLO101/0417	1
Fagron	Propionato de clobetasol	Clo103/0220	1
Fagron	Propionato de clobetasol	CLO103/0220	1
Fagron	Propionato de clobetasol	CLO103/0518	3
Fagron	Propionato de clobetasol	CLO105/0519	1
Fagron	Propionato de clobetasol	CLO111/1018	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propionato de clobetasol	CL0113/0619	5
Fagron	Propionato de clobetasol	CL04645878	1
Fagron	Propionato de clobetasol	F02-3653202	2
Fagron	Propionato de clobetasol	F02-3669401	1
Fagron	Propionato de clobetasol	F02-3669403	2
Fagron	Propionato de clobetasol	NS0292-M	1
Fagron	Propionato de clobetasol	NS0486M	1
Fagron	Propionato de clobetasol	NT0421M	3
Fargon/Phoenix 23.01.2018	Propionato de clobetasol	17E04-B02-338441	1
Fargon	Propionato de clobetasol	14C03-B07	1
Farmabios / Gehe	Propionato de clobetasol	15234003	1
Farmabios / Gehe	Propionato de clobetasol	18082703	1
Farmabios S.p.A./Cae...	Propionato de clobetasol	14338006	1
Farmabios S.p.A.	Propionato de clobetasol	18300204	1
Farmabios S.p.A/AHD	Propionato de clobetasol	18082708	1
Farmabios S.p.A/AHD	Propionato de clobetasol	18082718	1
Fgaron	Propionato de clobetasol	15H26-B03	1
fgron Services B.V./ Gehe	Propionato de clobetasol	F02-3669401	1
Fiebig	Propionato de clobetasol	1804002-01	1
Finteler Apotheke	Propionato de clobetasol	16K24-B04-333121	2
Fischar	Propionato de clobetasol	14188506	1
GEHE 21.03.2014	Propionato de clobetasol	1211021-02	1
Gehe amax	Propionato de clobetasol	15439501	1
Gehe amax	Propionato de clobetasol	18300204	1
Gehe/Euroh	Propionato de clobetasol	190301401	1
Gehe	Propionato de clobetasol	10D21-N04	1
Gehe	Propionato de clobetasol	12107606	1
Gehe	Propionato de clobetasol	12342306	2
Gehe	Propionato de clobetasol	12342310	1
Gehe	Propionato de clobetasol	12J25-N01	1
Gehe	Propionato de clobetasol	1408018-02	1
Gehe	Propionato de clobetasol	1408018-03	1
Gehe	Propionato de clobetasol	14188504	1
Gehe	Propionato de clobetasol	15234003	1
Gehe	Propionato de clobetasol	1606022-01	2
Gehe	Propionato de clobetasol	16106701	1
Gehe	Propionato de clobetasol	16106704	1
GEHE	Propionato de clobetasol	16G18-B02-324627	1
Gehe	Propionato de clobetasol	170402001	1
Gehe	Propionato de clobetasol	1704020-01	1
Gehe	Propionato de clobetasol	17096705	1
GEHE	Propionato de clobetasol	17096707	1
Gehe	Propionato de clobetasol	17096708	1
Gehe	Propionato de clobetasol	1804002-01	1
GEHE	Propionato de clobetasol	18082702	1
Gehe	Propionato de clobetasol	18082703	1
Gehe	Propionato de clobetasol	183002001	2
Gehe	Propionato de clobetasol	18I12-B02-353203	1
Gehe	Propionato de clobetasol	18I12-B02-355391	1
Gehe	Propionato de clobetasol	1903014-01	2
Gehe	Propionato de clobetasol	20004302009	1
GEHE	Propionato de clobetasol	210017000003	1
Gehe	Propionato de clobetasol	21001700013	1
Gehe	Propionato de clobetasol	21001700018	1
Gehe	Propionato de clobetasol	21001700025	2
Gehe	Propionato de clobetasol	2100700026	1
Gehe	Propionato de clobetasol	2109003-01	1
GEHE	Propionato de clobetasol	2209014_01	1
Gehe	Propionato de clobetasol	2209014-01	1
GEHE	Propionato de clobetasol	22H25-B08-223090	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Propionato de clobetasol	23000426002	2
Gehe	Propionato de clobetasol	23000426003	1
Gehe	Propionato de clobetasol	23003315001	1
gehe	Propionato de clobetasol	APCLPM03616C	1
gehe	Propionato de clobetasol	Fagron23D-01B01-227673	1
Geilenkirchen	Propionato de clobetasol	18082703	1
Geilenkirchen	Propionato de clobetasol	192245011	1
Geilenkirchen	Propionato de clobetasol	210017000003	1
HCK	Propionato de clobetasol	11/05-N06	1
Hedinger/ Sanacorp	Propionato de clobetasol	APAPL/035/E-12C	1
Hedinger	Propionato de clobetasol	1704020-01	1
Henry Lamotte	Propionato de clobetasol	16106704	1
Heyl/Noweda	Propionato de clobetasol	15234001	2
Ichtyol / Noweda	Propionato de clobetasol	17325605	1
Jenapharm/Noweda	Propionato de clobetasol	15234004	1
Jenne	Propionato de clobetasol	17325601	2
Jenne	Propionato de clobetasol	21001700001	1
Jenne	Propionato de clobetasol	21001700013	5
Jenne	Propionato de clobetasol	22H25-B0B-225386	1
Kehr	Propionato de clobetasol	22000315001	1
Kehr	Propionato de clobetasol	23000426001	1
Kehr	Propionato de clobetasol	2300042600214	1
Krieger	Propionato de clobetasol	2209014-01	1
L10	Propionato de clobetasol	16106703	2
L10	Propionato de clobetasol	18082708	1
L12	Propionato de clobetasol	16106711	1
L12	Propionato de clobetasol	17325602	1
Midas	Propionato de clobetasol	16106704	2
Midas	Propionato de clobetasol	17096705	1
Nachprüfung vom 19.06.17	Propionato de clobetasol	9302004	2
Nachprüfung	Propionato de clobetasol	2082019-11	1
Newchem / Gehe	Propionato de clobetasol	17096708	1
Newchem S.p.A./Link	Propionato de clobetasol	NZ0263M/X2835	1
Newchem S.p.A.	Propionato de clobetasol	192245008	1
Newchem/Phoenix	Propionato de clobetasol	NZ0263M	2
Newchem	Propionato de clobetasol	15439504	2
Noweda /Cealo	Propionato de clobetasol	18300209	1
Noweda 6.4.17	Propionato de clobetasol	1606022-01	1
Noweda/ Ichthyol	Propionato de clobetasol	15439503	1
Noweda/Anzag	Propionato de clobetasol	13269504	3
Noweda/EuRo	Propionato de clobetasol	1606022-01	1
Noweda	Propionato de clobetasol	11300702	1
Noweda	Propionato de clobetasol	12342305	1
Noweda	Propionato de clobetasol	12342310	1
Noweda	Propionato de clobetasol	13134701	1
Noweda	Propionato de clobetasol	13134705	1
Noweda	Propionato de clobetasol	14338007	1
Noweda	Propionato de clobetasol	15234004	1
Noweda	Propionato de clobetasol	1606022-02	1
Noweda	Propionato de clobetasol	16106720	1
Noweda	Propionato de clobetasol	17096706	1
Noweda	Propionato de clobetasol	17325605	1
Noweda	Propionato de clobetasol	17G14-B12-340175	1
Noweda	Propionato de clobetasol	1804002-01	2
Noweda	Propionato de clobetasol	18300202	1
Noweda	Propionato de clobetasol	18300204	1
Noweda	Propionato de clobetasol	18300208	1
Noweda	Propionato de clobetasol	18300213	1
Noweda	Propionato de clobetasol	1903014-01	2
Noweda	Propionato de clobetasol	192245003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Propionato de clobetasol	20004302006	1
Noweda	Propionato de clobetasol	2005025-01	3
Noweda	Propionato de clobetasol	21001700003	1
Noweda	Propionato de clobetasol	21001700023	1
Noweda	Propionato de clobetasol	21001700025	1
Noweda	Propionato de clobetasol	2109003-01	3
Noweda	Propionato de clobetasol	2209014-01	1
Noweda	Propionato de clobetasol	22H25-B08-223090	1
Noweda	Propionato de clobetasol	23000426001	2
NOWEDA	Propionato de clobetasol	23000426001	1
Oberlinden Apotheke	Propionato de clobetasol	B0054/116010Mg60g	1
Parthe Apotheke	Propionato de clobetasol	96/21	1
Ph.Eur 8.0	Propionato de clobetasol	16106709	1
Phoenix 02.04.2014	Propionato de clobetasol	1211021-03	3
Phoenix 24.11.2017	Propionato de clobetasol	17096706	1
Phoenix 29.11.12	Propionato de clobetasol	700225	2
Phoenix WE 29.04.17 ...	Propionato de clobetasol	1606022-02	1
Phoenix/Cealo	Propionato de clobetasol	17096701	1
phoenix/fargon	Propionato de clobetasol	17L18-B02-345403	1
Phoenix	Propionato de clobetasol	13K08B30287728	1
Phoenix	Propionato de clobetasol	15439502	1
Phoenix	Propionato de clobetasol	16h22-b07-328012	1
Phoenix	Propionato de clobetasol	16H-B07-330169	1
Phoenix	Propionato de clobetasol	1704020-01	1
Phoenix	Propionato de clobetasol	1804002-01	1
Phoenix	Propionato de clobetasol	18082703	2
Phoenix	Propionato de clobetasol	18082709	1
Phoenix	Propionato de clobetasol	183002001	1
Phoenix	Propionato de clobetasol	1903014-01	2
Phoenix	Propionato de clobetasol	192245002	1
Phoenix	Propionato de clobetasol	192245011	1
Phoenix	Propionato de clobetasol	20004302002	1
Phoenix	Propionato de clobetasol	20004302003	2
Phoenix	Propionato de clobetasol	200451305	1
Phoenix	Propionato de clobetasol	21001700007	1
Phoenix	Propionato de clobetasol	2100170003	1
Phoenix	Propionato de clobetasol	2109003-01	1
Phoenix	Propionato de clobetasol	2209014-01	1
Phoenix	Propionato de clobetasol	22H25-B08-223090	1
Phoenix	Propionato de clobetasol	23000426001	3
Phoenix	Propionato de clobetasol	23000426003	1
Phoenix	Propionato de clobetasol	3063	1
Phoenix	Propionato de clobetasol	3365	1
Phoenix	Propionato de clobetasol	3366	1
Phönix Caesar u. Loretz	Propionato de clobetasol	13269508	1
Phönix Gotha	Propionato de clobetasol	1108044-04	1
Phönix Gotha	Propionato de clobetasol	1211021-02	3
Phönix Gotha	Propionato de clobetasol	18082708	1
phönix herne	Propionato de clobetasol	180400201	1
Phönix, Caesar&Loret...	Propionato de clobetasol	18300213	1
Phönix/Apo-Ident	Propionato de clobetasol	1606022-02	1
Phönix/Euro	Propionato de clobetasol	1804002-01	1
Phönix	Propionato de clobetasol		1
Phönix	Propionato de clobetasol	1211021-04	1
Phönix	Propionato de clobetasol	13134701	1
phönix	Propionato de clobetasol	15439503	1
phönix	Propionato de clobetasol	15439504	1
Phönix	Propionato de clobetasol	15H26-B03-312860	1
Phönix	Propionato de clobetasol	16106703	1
phönix	Propionato de clobetasol	16106704	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Propionato de clobetasol	17096706	2
Phönix	Propionato de clobetasol	1804002-01	1
phönix	Propionato de clobetasol	18082703	1
Phönix	Propionato de clobetasol	18300204	1
Phönix	Propionato de clobetasol	192245004	1
Phönix	Propionato de clobetasol	20004302002	1
Phönix	Propionato de clobetasol	2002025-01	1
Phönix	Propionato de clobetasol	200990910	1
Phönix	Propionato de clobetasol	21001700026	1
Phönix	Propionato de clobetasol	2109003-01	1
Phönix	Propionato de clobetasol	3161	1
Phönix	Propionato de clobetasol	3182	1
Phönix	Propionato de clobetasol	F02-3653202	1
PhönixWE24.10.2014 …	Propionato de clobetasol	1211021-04	1
Raben-Apotheke Mildenau	Propionato de clobetasol	13k08-b30-287727	1
Röntgen	Propionato de clobetasol	1804002-01	1
Sanacorp	Propionato de clobetasol	1108044-03	1
Sanacorp	Propionato de clobetasol	12107608	1
Sanacorp	Propionato de clobetasol	12107609	2
Sanacorp	Propionato de clobetasol	1211021-01	1
Sanacorp	Propionato de clobetasol	12342310	1
Sanacorp	Propionato de clobetasol	13269507	1
sanacorp	Propionato de clobetasol	13269508	1
Sanacorp	Propionato de clobetasol	13g23n01	1
sanacorp	Propionato de clobetasol	14188506	1
Sanacorp	Propionato de clobetasol	15234003	1
Sanacorp	Propionato de clobetasol	1606022-02	2
Sanacorp	Propionato de clobetasol	18082708	1
Sanacorp	Propionato de clobetasol	18300204	1
Sanacorp	Propionato de clobetasol	18I12-B02_357669	1
Sanacorp	Propionato de clobetasol	192245004	1
Sanacorp	Propionato de clobetasol	20004302009	1
Sanacorp	Propionato de clobetasol	2005025-01	1
Sanacorp	Propionato de clobetasol	21001700003	2
Sanacorp	Propionato de clobetasol	21001700023	1
Sanacorp	Propionato de clobetasol	21L16-B08-221088	1
Sanacorp	Propionato de clobetasol	230003315003	1
Sanacorp	Propionato de clobetasol	23000426001	2
sanacorp	Propionato de clobetasol	23000426002	1
Sanacorp;19.03.15;87,60EUR	Propionato de clobetasol	14C03-B07-293563	1
Symbiotica / Gehe	Propionato de clobetasol	1408018-02	1
Symbiotica / Gehe	Propionato de clobetasol	1408018-03	2
Symbiotica / Noweda	Propionato de clobetasol	1704020-01	1
Symbiotica Spec. Ing…	Propionato de clobetasol	19J02-F02-365322	1
Symbiotica Spec./Phönix	Propionato de clobetasol	1108044-04	1
Symbiotica Spec./Phönix	Propionato de clobetasol	CLO-B12153/0711	1
Symbiotica Spec.	Propionato de clobetasol	1211021-03	1
symbiotica/gehe	Propionato de clobetasol	1211021-03	1
Symbiotica/Noweda	Propionato de clobetasol	CLO119/1217	1
Symbiotica/Phönix	Propionato de clobetasol	1408018-02	1
Symbiotica/Sanacorp	Propionato de clobetasol	1408018-03	1
Symbiotica	Propionato de clobetasol	2005025-01	2
symbiotica	Propionato de clobetasol	2109003	1
Symbiotica	Propionato de clobetasol	2109003-01	1
Symbiotitica/Noweda	Propionato de clobetasol	1606022-01	1
VDL	Propionato de clobetasol	2109003-01	1
WE: 20.01.16	Propionato de clobetasol	15234004	1

- 231 623 spectra from 1513 *Apo-Ident* customers from a total of 48 653 batches from a further

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Propionato de clobetasol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propionato de clobetasol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	740	0	152 222
Type B	0	1184	0	200 900
Type C	0	4346	98	231 623

The substance/substance group *Propionato de clobetasol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1892 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4932 %)
Type C	100.0000 % (> 99.9007 %)	97.7948 % (> 97.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21092	21092	0,00	75,82
21473	21473	0,00	55,71
21611	21611	0,00	54,44
21802	21802	0,00	114,52
21896	21896	0,00	79,38
22714	22714	0,00	54,21
22724	21092	5,98	74,93
24691	25349	8,08	53,48
24904	24904	0,00	80,40
25349	25349	0,00	52,73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Propionato de testosterona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20880-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propionato de testosterona; Testosterona, propionato; Testosteroni propionas

Special notes

When selecting the *Propionato de testosterona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Propionato de testosterona	6	11	278

Second-stage model

For differentiation of the substance/substance group *Propionato de testosterona* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Propionato de testosterona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Progesterona	37,34	48,82
Espironolactona	49,58	49,67
⋮	⋮	⋮
Iodopovidona	>50	84,15
Povidona	>50	84,83
Ácido fusídico	>50	114,35
Ubidecarenona	>50	127,06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Propionato de testosterona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Propionato de testosterona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propionato de testosterona	12163607	20880	40	AR-15-FG-000623-01
Caelo	Propionato de testosterona	15444709	23170	40	1707612
Euro OTC	Propionato de testosterona	1109024-02	21644	60	1503607
Euro OTC	Propionato de testosterona	1511003	22230	60	20151111*
Euro OTC	Propionato de testosterona	1511003	22230SI	43	20151111*
Euro OTC	Propionato de testosterona	1512023	22288	45	20151230*
Euro OTC	Propionato de testosterona	1512023	22288SI	45	20151230*
Euro OTC	Propionato de testosterona	2003011	25116	40	20200408*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 373 spectra of 8 reference samples from the substance/substance group *Propionato de testosterona*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 589 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 939 spectra of 24 reference samples from the substance/substance group *Propionato de testosterona*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propionato de testosterona	170963	23334	40
Caelo	Propionato de testosterona	191986	24759	40
Caelo	Propionato de testosterona	22003581	26494	40
Caelo	Propionato de testosterona	23001951	26952	40
Euro OTC	Propionato de testosterona	1710027	23734	40
Euro OTC	Propionato de testosterona	1811040	24413	40
Euro OTC	Propionato de testosterona	2010004	25476	40
Euro OTC	Propionato de testosterona	2206019	26205	40
Euro OTC	Propionato de testosterona	2309024	26925	40
Fagron	Propionato de testosterona	22F07-F03-382822	26373	40
Fagron	Propionato de testosterona	24E02-B03-241020	27411	40
Caelo	Propionato de testosterona	15444709	23170SI†	30
Caelo	Propionato de testosterona	170963	23334SI	29
Caelo	Propionato de testosterona	191986	24759SI	40
Caelo	Propionato de testosterona	22003581	26494SI	40
Caelo	Propionato de testosterona	23001951	26952SI	40
Euro OTC	Propionato de testosterona	1710027	23734SI	40
Euro OTC	Propionato de testosterona	1811040	24413SI	40
Euro OTC	Propionato de testosterona	2003011	25116SI†	40
Euro OTC	Propionato de testosterona	2010004	25476SI	40
Euro OTC	Propionato de testosterona	2206019	26205SI	40
Euro OTC	Propionato de testosterona	2309024	26925SI	40
Fagron	Propionato de testosterona	22F07-F03-382822	26373SI	40
Fagron	Propionato de testosterona	24E02-B03-241020	27411SI	40

- 201 145 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 934 spectra from 428 *Apo-Ident* customers from 294 batches from the substance/substance group *Propionato de testosterona*.

- Among them are spectra of independent samples from 278 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Propionato de testosterona	16C24-B04-320784	2
	Propionato de testosterona	2010004-02	1
	Propionato de testosterona	2206019-01	1
	Propionato de testosterona	2206019-02	4
	Propionato de testosterona	22K07-B09	1
	Propionato de testosterona	22K07-B09-223645	2
	Propionato de testosterona	22K07-b09-223647	1
	Propionato de testosterona	22K07-B09-223647	6
	Propionato de testosterona	22K07-B09-228637	7
	Propionato de testosterona	23J09-B10-233051	2
	Propionato de testosterona	f03-3828201	1
	Propionato de testosterona	TSP103/0322	2
AHD	Propionato de testosterona	17325712	1
AHD	Propionato de testosterona	19K11-F05	1
AHD	Propionato de testosterona	AP12E04-N01TP	1
AHL	Propionato de testosterona	APZTSP15003-MTP	2
Alliance	Propionato de testosterona	2206019-02	1
Alliance	Propionato de testosterona	22k07-b09-223645	1
allianz	Propionato de testosterona	15444704	1
Andor	Propionato de testosterona	1109024-03TP	1
Anzag	Propionato de testosterona	14L31-B02-304722	1
Anzag	Propionato de testosterona	20K26-F06-375792	1
Apo-ident / AH	Propionato de testosterona	2003011-01	1
apomix	Propionato de testosterona	13K25-B05-287648	1
apomix	Propionato de testosterona	40/14	1
Audor Pharma	Propionato de testosterona	AP1109024-03	2
Audor Pharma	Propionato de testosterona	AP1109024-03TP	4
Audor Pharma	Propionato de testosterona	AP12E04N01TP	2
Audor Pharma	Propionato de testosterona	AP12J10-N08TP	2
Audor Pharma	Propionato de testosterona	AP13K25-B05-287643T	1
Audor Pharma	Propionato de testosterona	AP13K25-B05-287643TP	1
Audor Pharma	Propionato de testosterona	APZTSP15003-MTP	16
Audor Pharma	Propionato de testosterona	APZTSP1503-MTP	1
Caelo	Propionato de testosterona	10235809	1
Caelo	Propionato de testosterona	103004	1
Caelo	Propionato de testosterona	106212376	1
Caelo	Propionato de testosterona	1108212376	1
Caelo	Propionato de testosterona	1109024-02	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propionato de testosterona	12060102	2
Caelo	Propionato de testosterona	12163605	2
Caelo	Propionato de testosterona	12163607	1
Caelo	Propionato de testosterona	12163610	2
Caelo	Propionato de testosterona	12163612	6
Caelo	Propionato de testosterona	12163613	1
Caelo	Propionato de testosterona	12163615	2
Caelo	Propionato de testosterona	12163616	4
Caelo	Propionato de testosterona	12163617	4
Caelo	Propionato de testosterona	12163619	2
Caelo	Propionato de testosterona	12163621	1
Caelo	Propionato de testosterona	1263607	1
Caelo	Propionato de testosterona	12A02-N05	1
Caelo	Propionato de testosterona	12J10-N08	2
Caelo	Propionato de testosterona	13C08-N02	1
Caelo	Propionato de testosterona	13F05-N04	1
Caelo	Propionato de testosterona	13K25-B05-291974	1
Caelo	Propionato de testosterona	14D15-B03-296959	1
Caelo	Propionato de testosterona	14L31-B02-304722	2
Caelo	Propionato de testosterona	15003002	8
Caelo	Propionato de testosterona	15003004	3
Caelo	Propionato de testosterona	15003008	2
Caelo	Propionato de testosterona	151100301	1
Caelo	Propionato de testosterona	1511003-01	1
Caelo	Propionato de testosterona	15169504	1
Caelo	Propionato de testosterona	15444702	10
Caelo	Propionato de testosterona	15444703	16
Caelo	Propionato de testosterona	15444705	4
Caelo	Propionato de testosterona	15444706	3
Caelo	Propionato de testosterona	15444707	4
Caelo	Propionato de testosterona	15444709	1
Caelo	Propionato de testosterona	15444710	5
Caelo	Propionato de testosterona	15444711	1
Caelo	Propionato de testosterona	15444712	1
Caelo	Propionato de testosterona	15444713	2
Caelo	Propionato de testosterona	15444714	3
Caelo	Propionato de testosterona	15444717	1
Caelo	Propionato de testosterona	15444718	2
Caelo	Propionato de testosterona	15444719	1
Caelo	Propionato de testosterona	15444721	2
Caelo	Propionato de testosterona	15444723	1
Caelo	Propionato de testosterona	1544717	1
Caelo	Propionato de testosterona	16E24-B01-324711	2
Caelo	Propionato de testosterona	16H22-B05-326483	1
Caelo	Propionato de testosterona	1710027-01	2
Caelo	Propionato de testosterona	17325707	10
Caelo	Propionato de testosterona	17325709	2
Caelo	Propionato de testosterona	17325711	2
Caelo	Propionato de testosterona	17325712	2
Caelo	Propionato de testosterona	17325712P-190312-8	1
Caelo	Propionato de testosterona	17325716	1
Caelo	Propionato de testosterona	17325717	9
Caelo	Propionato de testosterona	17325719	2
Caelo	Propionato de testosterona	17B09B03332376	1
Caelo	Propionato de testosterona	17B09-B03-332376	1
Caelo	Propionato de testosterona	17J16-B03-341320	1
Caelo	Propionato de testosterona	18b06-B04	1
Caelo	Propionato de testosterona	18b06-b04-351510	1
Caelo	Propionato de testosterona	18B14-B02-353456	1
Caelo	Propionato de testosterona	18I12-B03-355137	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propionato de testosterona	191986001	3
Caelo	Propionato de testosterona	191986003	1
Caelo	Propionato de testosterona	191986007	2
Caelo	Propionato de testosterona	19198603	6
Caelo	Propionato de testosterona	19198603P-200319-13	1
Caelo	Propionato de testosterona	19198604	8
Caelo	Propionato de testosterona	19k11-f05-366325	1
Caelo	Propionato de testosterona	2013U-02376	1
Caelo	Propionato de testosterona	20H19-F07-373643	1
Caelo	Propionato de testosterona	21000430001	1
Caelo	Propionato de testosterona	21000430002	3
Caelo	Propionato de testosterona	21000430006	2
Caelo	Propionato de testosterona	21000430010	1
Caelo	Propionato de testosterona	22003581002	3
Caelo	Propionato de testosterona	22K07-B09-223647	1
Caelo	Propionato de testosterona	23051816	1
Caelo	Propionato de testosterona	2910030-02	1
Caelo	Propionato de testosterona	36814m1	1
Caelo	Propionato de testosterona	36814M1	2
Caelo	Propionato de testosterona	612212376	1
Caelo	Propionato de testosterona	614E2376	1
Caelo	Propionato de testosterona	903312376	1
Caesar & Loretz GmbH...	Propionato de testosterona	17325719	1
Caesar & Loretz GmbH...	Propionato de testosterona	19198603	1
Caesar & Loretz GmbH...	Propionato de testosterona	21000430006	2
Caesar & Loretz GmbH...	Propionato de testosterona	17325722	1
Caesar & Loretz GmbH...	Propionato de testosterona	19198604	2
Caesar & Loretz GmbH	Propionato de testosterona	17325716	1
Caesar & Loretz GmbH	Propionato de testosterona	17325717	2
CAESAR & LORETZ GMBH	Propionato de testosterona	191986003	2
Caesar & Loretz GmbH	Propionato de testosterona	191986006	1
Caesar & Loretz GmbH	Propionato de testosterona	19198603	2
Caesar & Loretz GmbH	Propionato de testosterona	19198604	5
Caesar & Loretz GmbH	Propionato de testosterona	21000430002	1
Caesar & Loretz GmbH	Propionato de testosterona	21000430006	1
Caesar & Loretz GmbH	Propionato de testosterona	21000430009	3
Caesar & Loretz GmbH	Propionato de testosterona	21000430010	1
Caesar & Loretz GmbH	Propionato de testosterona	21000430012	2
Caesar & Loretz GmbH	Propionato de testosterona	22003581003	1
Ebert 17.08.16	Propionato de testosterona	15444703	1
EURHO/Anzag	Propionato de testosterona	1811040-01	1
EuRho/Krieger	Propionato de testosterona	1811040-01	3
EuRho	Propionato de testosterona	17100271	1
EuRho	Propionato de testosterona	1811040-01	1
EuRho	Propionato de testosterona	2003011-01	1
Euro OTC	Propionato de testosterona	101/0218	1
Euro OTC	Propionato de testosterona	1103010-01	1
Euro OTC	Propionato de testosterona	1103010-02	1
Euro OTC	Propionato de testosterona	1109024-02	1
Euro OTC	Propionato de testosterona	1109024-03	1
Euro OTC	Propionato de testosterona	1409037-01	2
Euro OTC	Propionato de testosterona	1504023-01	5
Euro OTC	Propionato de testosterona	1511003-01	10
Euro OTC	Propionato de testosterona	1512023-01	2
Euro OTC	Propionato de testosterona	15444718	2
Euro OTC	Propionato de testosterona	1710027-01	8
Euro OTC	Propionato de testosterona	181040-01	1
Euro OTC	Propionato de testosterona	181104001	2
Euro OTC	Propionato de testosterona	1811040-01	16
Euro OTC	Propionato de testosterona	18111709	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Propionato de testosterona	18114001	1
Euro OTC	Propionato de testosterona	2003011-01	10
Euro OTC	Propionato de testosterona	2010004-01	14
Euro OTC	Propionato de testosterona	2010004-02	1
Euro OTC	Propionato de testosterona	710027-01	1
Euro OTC	Propionato de testosterona	970116/1	1
Euro OTC	Propionato de testosterona	F07-3736403	1
Euro/Lui	Propionato de testosterona	1811040-01	1
euro	Propionato de testosterona	2010004-01	1
Fagro/Noweda	Propionato de testosterona	16H22-B05-326483	2
Fagron	Propionato de testosterona		2
Fagron	Propionato de testosterona	10L03-N16	3
Fagron	Propionato de testosterona	11/12-N03	1
Fagron	Propionato de testosterona	11C21-N09	1
Fagron	Propionato de testosterona	11G15-N07	3
Fagron	Propionato de testosterona	11K18-N04	4
Fagron	Propionato de testosterona	12/10-N08	1
Fagron	Propionato de testosterona	12163616	2
Fagron	Propionato de testosterona	12A02-N05	2
Fagron	Propionato de testosterona	12C01-N01	1
Fagron	Propionato de testosterona	12C01-NO1	1
Fagron	Propionato de testosterona	12E04-N01	3
Fagron	Propionato de testosterona	12E29-N02	1
Fagron	Propionato de testosterona	12J10N-08	1
Fagron	Propionato de testosterona	12J10-N08	4
Fagron	Propionato de testosterona	13/03-N02	2
Fagron	Propionato de testosterona	13C08N02	1
Fagron	Propionato de testosterona	13C08-N02	15
Fagron	Propionato de testosterona	13F05-N04	16
Fagron	Propionato de testosterona	13I03-N02	1
Fagron	Propionato de testosterona	13K25-B05	1
Fagron	Propionato de testosterona	13K25-B05-287647	10
Fagron	Propionato de testosterona	13K25B05287648	1
Fagron	Propionato de testosterona	13K25-B05-287648	5
Fagron	Propionato de testosterona	13K25-B05-291974	2
Fagron	Propionato de testosterona	14A28-B12	2
Fagron	Propionato de testosterona	14A28-B12-291977	1
Fagron	Propionato de testosterona	14A28B12296958	1
Fagron	Propionato de testosterona	14A28-B12-296958	2
Fagron	Propionato de testosterona	14A28-B12-296960	2
Fagron	Propionato de testosterona	14D15-B03-296959	4
Fagron	Propionato de testosterona	14l31-B02	1
Fagron	Propionato de testosterona	14L31-B02	4
Fagron	Propionato de testosterona	14L31B02-304721	1
Fagron	Propionato de testosterona	14L31-B02-304721	9
Fagron	Propionato de testosterona	14L31B02304722	1
Fagron	Propionato de testosterona	14L31-B02-304722	11
Fagron	Propionato de testosterona	15/01-B09	1
Fagron	Propionato de testosterona	15/01-B09-312867	1
Fagron	Propionato de testosterona	15/01-B09-318371	2
Fagron	Propionato de testosterona	1501-B09-312867	1
Fagron	Propionato de testosterona	1511003-01	1
Fagron	Propionato de testosterona	15444717	1
Fagron	Propionato de testosterona	15D03-B02-310694	1
Fagron	Propionato de testosterona	15I01-B01-318371	1
Fagron	Propionato de testosterona	15I01-B09-312867	2
Fagron	Propionato de testosterona	15I01-B09-318371	2
Fagron	Propionato de testosterona	15k03-b03	1
Fagron	Propionato de testosterona	15K03-B03-315218	7
Fagron	Propionato de testosterona	15K03-B-03-315218	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propionato de testosterona	15101-B09-312867	1
Fagron	Propionato de testosterona	16C24B04320784	1
Fagron	Propionato de testosterona	16C24-B04-320784	4
Fagron	Propionato de testosterona	16E24-B01	1
Fagron	Propionato de testosterona	16E24-B01-322593	7
Fagron	Propionato de testosterona	16E24B01322938	1
Fagron	Propionato de testosterona	16E24B01324711	1
Fagron	Propionato de testosterona	16E24-B01-324711	2
Fagron	Propionato de testosterona	16E24-B01-325476	1
Fagron	Propionato de testosterona	16E24-Bo1-322938	1
Fagron	Propionato de testosterona	16H22-B05	2
Fagron	Propionato de testosterona	16H22-B05-326482	4
Fagron	Propionato de testosterona	16h22-b05-326483	1
Fagron	Propionato de testosterona	16H22B05326483	1
Fagron	Propionato de testosterona	16H22-B05-326483	12
Fagron	Propionato de testosterona	16K24B03330544	1
Fagron	Propionato de testosterona	16K24-B03-330544	1
Fagron	Propionato de testosterona	17116-B04-346529	1
Fagron	Propionato de testosterona	17B09-B03	1
Fagron	Propionato de testosterona	17B09B03332376	1
Fagron	Propionato de testosterona	17B09-B03-332376	6
Fagron	Propionato de testosterona	17B09-B04-335269	2
Fagron	Propionato de testosterona	17E22-B09	1
Fagron	Propionato de testosterona	17E22-B09-338592	4
Fagron	Propionato de testosterona	17H25-B02-341321	4
Fagron	Propionato de testosterona	17J16-B03	1
Fagron	Propionato de testosterona	17j16-B03-341320	1
Fagron	Propionato de testosterona	17J16B03-341320	2
Fagron	Propionato de testosterona	17J16-B03-341320	1
Fagron	Propionato de testosterona	17J16-B03-343010	4
Fagron	Propionato de testosterona	17J16-B03-344243	2
Fagron	Propionato de testosterona	17J16B04346529	1
Fagron	Propionato de testosterona	17J16-B04-346529	7
Fagron	Propionato de testosterona	18/12-B03	1
Fagron	Propionato de testosterona	18/12-B03-355296	2
Fagron	Propionato de testosterona	18/12-B03-3567	1
Fagron	Propionato de testosterona	18/12-B03-356702	4
Fagron	Propionato de testosterona	18/12-B03-356703	4
Fagron	Propionato de testosterona	18/12-B03-3596	1
Fagron	Propionato de testosterona	18B06-B04	2
Fagron	Propionato de testosterona	18B06-B04-348557	4
Fagron	Propionato de testosterona	18B06B04350560	1
Fagron	Propionato de testosterona	18B06-B04-350560	1
Fagron	Propionato de testosterona	18B06-B04-351510	7
Fagron	Propionato de testosterona	18B06-B04-352492	4
Fagron	Propionato de testosterona	18B06-B04-352493	6
Fagron	Propionato de testosterona	18b14-b02-353456	1
Fagron	Propionato de testosterona	18B14-B02-353456	2
Fagron	Propionato de testosterona	18I12-B03	1
Fagron	Propionato de testosterona	18I12-B03-355137	2
Fagron	Propionato de testosterona	18I12-B03-355296	2
Fagron	Propionato de testosterona	18I12-B03-356702	1
Fagron	Propionato de testosterona	18I12-B03-356703	2
Fagron	Propionato de testosterona	18I22-B03-356703	1
Fagron	Propionato de testosterona	18l12-B03-356703	1
Fagron	Propionato de testosterona	19H16-F03-364849	4
Fagron	Propionato de testosterona	19H16-F03-364850	7
Fagron	Propionato de testosterona	19H22-B05-326483	1
Fagron	Propionato de testosterona	19K11-F05-366324	9
Fagron	Propionato de testosterona	19K11-F05-366325	11

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propionato de testosterona	20121012-3	1
Fagron	Propionato de testosterona	20A27-F08	2
Fagron	Propionato de testosterona	20A27-F08-368802	6
Fagron	Propionato de testosterona	20A27-F08-368803	1
Fagron	Propionato de testosterona	20A27-F08-368803	2
Fagron	Propionato de testosterona	20A27F08369542	1
Fagron	Propionato de testosterona	20A27-F08-369542	2
Fagron	Propionato de testosterona	20F24-F02	1
Fagron	Propionato de testosterona	20F24-F02-371915	7
Fagron	Propionato de testosterona	20F24-F02-371916	10
Fagron	Propionato de testosterona	20F24-FO2-371915	1
Fagron	Propionato de testosterona	20H19-F07	2
Fagron	Propionato de testosterona	20H19-F07-3736403	1
Fagron	Propionato de testosterona	20H19-F07-373642	6
Fagron	Propionato de testosterona	20H19-F07-373643	9
Fagron	Propionato de testosterona	20H19-F07-373643	1
Fagron	Propionato de testosterona	20H19-F07-375282	4
Fagron	Propionato de testosterona	20K26-F06	3
Fagron	Propionato de testosterona	20K26-F06-375792	6
Fagron	Propionato de testosterona	20K26-F06-375793	7
Fagron	Propionato de testosterona	21J04-F03	2
Fagron	Propionato de testosterona	21J04F03-380627	1
Fagron	Propionato de testosterona	21J04-F03-380627	8
Fagron	Propionato de testosterona	21J04-F03-380628	13
Fagron	Propionato de testosterona	21JO4-F03-380627	1
Fagron	Propionato de testosterona	22F07-03F-382821	1
Fagron	Propionato de testosterona	22F07-F03-382821	7
Fagron	Propionato de testosterona	22K07-B09	1
Fagron	Propionato de testosterona	22K07-B09-223647	1
Fagron	Propionato de testosterona	24411M1	1
Fagron	Propionato de testosterona	2OF24-FO2-371915	1
Fagron	Propionato de testosterona	2OK26-F06-375792	1
Fagron	Propionato de testosterona	2OK26-FO6-375792	1
Fagron	Propionato de testosterona	32012M1	1
Fagron	Propionato de testosterona	3380627	1
Fagron	Propionato de testosterona	3613M-02376	1
Fagron	Propionato de testosterona	36513M1	3
Fagron	Propionato de testosterona	36814M1	2
Fagron	Propionato de testosterona	6081201	1
Fagron	Propionato de testosterona	APZTSP15003-MTP	2
Fagron	Propionato de testosterona	F02-3719105	2
Fagron	Propionato de testosterona	F02-3719106	1
Fagron	Propionato de testosterona	F03-3648500	1
Fagron	Propionato de testosterona	F06-3757902	7
Fagron	Propionato de testosterona	F06-3757903	1
Fagron	Propionato de testosterona	F07-3736402	2
Fagron	Propionato de testosterona	F07-3736403	2
Fagron	Propionato de testosterona	F07-3752802	2
Fagron	Propionato de testosterona	F08-3688002	1
Fagron	Propionato de testosterona	F08-3688003	2
Fagron	Propionato de testosterona	T009/07109	2
Fagron	Propionato de testosterona	t011/072000	1
Fagron	Propionato de testosterona	TSP101/0720	1
Fagron	Propionato de testosterona	TSP102/0720	1
Fagron	Propionato de testosterona	TSP-BLT008/0719	1
Fagron	Propionato de testosterona	TSP-BLT011/0720	1
Fargon - Alliance He...	Propionato de testosterona	18/12-B03-356703	1
Fargon /Max Jenne	Propionato de testosterona	18I12-B03-355296	1
Fargon/ Phönix	Propionato de testosterona	18I12-B03-356703	1
Fargon/Kehr	Propionato de testosterona	17B09-B04-335269	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fargon	Propionato de testosterona	19K11-F05_366324	1
Fiebig	Propionato de testosterona	20F24-F02-371915	1
Fragon	Propionato de testosterona	21j04-F03-380628	1
Galderma	Propionato de testosterona	15K03-B03-315218	1
Gatt-Koller	Propionato de testosterona	1803006	1
Gatt-Koller	Propionato de testosterona	3478/09153915	1
Gatt-Koller	Propionato de testosterona	606213811	1
Gehe/Euro	Propionato de testosterona	1200318/151100301	1
Gehe/Fragon	Propionato de testosterona	17B09B03332376	1
Gehe	Propionato de testosterona	14A28B12296958	1
Gehe	Propionato de testosterona	15444706	1
Gehe	Propionato de testosterona	16H22-B05	1
GEHE	Propionato de testosterona	17325709	1
GEHE	Propionato de testosterona	17325712	1
Gehe	Propionato de testosterona	19H16-F03	1
Gehe	Propionato de testosterona	19H16-F03-364849	1
Gehe	Propionato de testosterona	19K11-F05-366325	1
Gehe	Propionato de testosterona	20K26-F06-375792	1
Gehe	Propionato de testosterona	22K07-B09-228637	1
Infectopharm/Phönix	Propionato de testosterona	18B06-B04-352493	1
Jenne	Propionato de testosterona	22003581003	1
Jenne	Propionato de testosterona	22K07-B09-228637	1
Kehr/Fargon	Propionato de testosterona	17J16-B03-344243	1
Kehr/Fargon	Propionato de testosterona	18/12-B03-355296	2
Kehr	Propionato de testosterona	2206019-01	1
Noweda	Propionato de testosterona	12163610	1
Noweda	Propionato de testosterona	1511003	1
Noweda	Propionato de testosterona	17B09-B03-332376	1
Noweda	Propionato de testosterona	21J04-F03-380627	3
Noweda	Propionato de testosterona	2206019-01	2
Noweda	Propionato de testosterona	22F07-F03-382821	1
Noweda	Propionato de testosterona	22K07-B09-223647	1
Noweda	Propionato de testosterona	22K07-B09-228637	1
Phoenix/Cealo	Propionato de testosterona	36814M1	1
Phoenix	Propionato de testosterona	1109024-02	1
phoenix	Propionato de testosterona	12163615	1
Phönix WE:25.04.16 E...	Propionato de testosterona	14L31-B02-304722	1
Phönix/ Fargon	Propionato de testosterona	16H22-B05-326483	3
Phönix/ Fargon	Propionato de testosterona	19H16-F03-364850	1
Phönix/Euro	Propionato de testosterona	110301002	1
Phönix	Propionato de testosterona	12163613	1
Phönix	Propionato de testosterona	12163617	1
Phönix	Propionato de testosterona	12J10-N08	1
Phönix	Propionato de testosterona	13C08-N02	1
Phönix	Propionato de testosterona	13K25-B05	1
Phönix	Propionato de testosterona	14L31-B02-304722	1
Phönix	Propionato de testosterona	15444702	1
Phönix	Propionato de testosterona	15444707	1
Phönix	Propionato de testosterona	15444710	1
PHÖNIX	Propionato de testosterona	15444720	1
Phönix	Propionato de testosterona	17325704	1
Phönix	Propionato de testosterona	20H19-F07-373643	1
Sanacorp 12.06.2019 6,70EUR	Propionato de testosterona	1710027-01	1
Sanacorp	Propionato de testosterona	13K25-B05	1
Sanacorp	Propionato de testosterona	14L31-B02-304721	2
Sanacorp	Propionato de testosterona	18B06-B0	1
Sanacorp	Propionato de testosterona	18I12-B03	1
Sanacorp	Propionato de testosterona	19H16-F03	1
Sanacorp	Propionato de testosterona	20A27-F09	1
Sanacorp	Propionato de testosterona	21J04-F03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Propionato de testosterona	22Fo7-F03-382822	1
Sanacorp	Propionato de testosterona	TSP103/0322	2
symbiotec	Propionato de testosterona	APZTSP15003-MTP	1
Symbiotica Speciality	Propionato de testosterona	15444702	2

- 235 133 spectra from 1515 *Apo-Ident* customers from a total of 48 966 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Propionato de testosterona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propionato de testosterona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	373	0	152 589
Type B	0	939	0	201 145
Type C	0	848	86	235 133

The substance/substance group *Propionato de testosterona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3914 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3610 %)
Type C	100.0000 % (> 99.9007 %)	90.7923 % (> 90.4711 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20880	20880	0,00	39,75
21644	21644	0,00	38,36

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22230	22230	0,00	38,89
22288	22288	0,00	38,65
23170	23170	0,00	37,34
25116	25116	0,00	41,90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Proteinato de prata**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20178-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Proteinato de prata; Argentum proteinicum

Special notes

When selecting the *Proteinato de prata* substance/substance group, the following information is displayed to the user:

- Nota sobre identificação da proteinato de prata: O acetiltanato de proteinato de prata é uma substância semelhante que não está incluída na base de dados. Pode ser necessário fazer uma análise de identidade adicional, por exemplo, o teste de identificação de acetil da Ph. Eur. 2.3.1 - não produz coloração azul.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Proteinato de prata	4	3	15

Second-stage model

For differentiation of the substance/substance group *Proteinato de prata* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Proteinato de prata* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	41,23	–
Sulfato de polimixina B	109,68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Proteinato de prata* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Proteinato de prata*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Proteinato de prata	190092	24559	40	20190221*
Caelo	Proteinato de prata	22000752	26126	30	20220511*
Fagron	Proteinato de prata	23D24-B08-229456	26820	40	20230512
Fagron	Proteinato de prata	23J19-B03-235267	27037	40	20231108

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 150 spectra of 4 reference samples from the substance/substance group *Proteinato de prata*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 812 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Proteinato de prata*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Proteinato de prata	21001315	25801	50
Caelo	Proteinato de prata	24001987	27430	40
Fagron	Proteinato de prata	24D17-B09-238717	27377	40
Caelo	Proteinato de prata	22000752	26126SI†	20
Fagron	Proteinato de prata	23D24-B08-229456	26820SI†	20
Fagron	Proteinato de prata	23J19-B03-235267	27037SI†	20

- 201 894 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 40 spectra from 34 *Apo-Ident* customers from 15 batches from the substance/substance group *Proteinato de prata*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Proteinato de prata	21001315005	1
	Proteinato de prata	22000752007	2
	Proteinato de prata	22001101018	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Proteinato de prata	22F22-B01-220214	3
	Proteinato de prata	23D24-B08-229465	1
	Proteinato de prata	PTOR22-0172	1
2206030-01	Proteinato de prata	2206030-01	1
Caelo	Proteinato de prata	22000752001	3
Caelo	Proteinato de prata	22000752003	6
Caelo	Proteinato de prata	22000752004	1
Caelo	Proteinato de prata	22000752005	1
Caelo	Proteinato de prata	22000752006	1
Caelo	Proteinato de prata	22000752007	2
Caesar & Loretz GmbH	Proteinato de prata	22000752001	3
Caesar & Loretz GmbH	Proteinato de prata	22000752003	1
Caesar & Loretz GmbH	Proteinato de prata	22000752007	2
Euro OTC	Proteinato de prata	2206030-01	1
Fagron	Proteinato de prata	22D14B06216102	1
Fagron	Proteinato de prata	22D14-B06-216102	1
Fagron	Proteinato de prata	22F22-B01-220214	3
Fagron	Proteinato de prata	PTOR22-0172	1
Gehe	Proteinato de prata	22000752005	1
Noweda	Proteinato de prata	22F22-B01-220214	1
Sanacorp	Proteinato de prata	23D24-B08-233762	1

- 236 027 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Proteinato de prata* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Proteinato de prata* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	150	0	152 812
Type B	0	190	0	201 894
Type C	0	40	0	236 027

The substance/substance group *Proteinato de prata* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 85.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24559	24559	0,00	50,75
26126	26126	0,00	30,91
26820	24559	17,73	43,68
27037	24559	15,53	53,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Quinolina amarela**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20456-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinolina amarela

Special notes

When selecting the *Quinolina amarela* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Quinolina amarela	6	3	57

Second-stage model

For differentiation of the substance/substance group *Quinolina amarela* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Quinolina amarela* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	61,11	–
⋮	⋮	⋮
Sacarina sódica	>50	25,96
Sulfato de atropina	>50	107,25
Furoato de mometasona	>50	110,07
Escina, hidrossolúvel	>50	122,51
Citrato monobásico de magnésio, hid…	>50	189,44
Cloridrato de propranolol	>50	212,25
Hidrocortisona	>50	251,29
Fenitoína	>50	375,31
Sorbato de potássio	>50	383,54
Orotato de cálcio di-hidratado	>50	434,29

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Quinolina amarela* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Quinolina amarela*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinolina amarela	12042010	20922	40	20120314
Caelo	Quinolina amarela	13109108	21305	40	1711481
Caelo	Quinolina amarela	17034101	23400	40	1709327
Caelo	Quinolina amarela	172277	23685	30	20171020*
Caelo	Quinolina amarela	172277	24812	40	20171020*
Caelo	Quinolina amarela	20002519012	26737	40	231105522
Caelo	Quinolina amarela	23002618	26962	40	20231103*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Quinolina amarela*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 692 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 6 reference samples from the substance/substance group *Quinolina amarela*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinolina amarela	16050101	23401	40
Caelo	Quinolina amarela	190734	24555	40
Fagron	Quinolina amarela	12E24-N01	20731	60
Caelo	Quinolina amarela	190734	24725	40
Caelo	Quinolina amarela	20002519012	26737SI†	20
Caelo	Quinolina amarela	23002618	26962SI†	20

- 201 864 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 179 spectra from 99 *Apo-Ident* customers from 60 batches from the substance/substance group *Quinolina amarela*.

- Among them are spectra of independent samples from 57 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Quinolina amarela	20002519008	1
	Quinolina amarela	20002519011	1
Caelo	Quinolina amarela	11089606	1
Caelo	Quinolina amarela	11089608	1
Caelo	Quinolina amarela	11089610	1
Caelo	Quinolina amarela	118E-03146	1
Caelo	Quinolina amarela	12042002	3
Caelo	Quinolina amarela	12042004	1
Caelo	Quinolina amarela	12042007	3
Caelo	Quinolina amarela	12042010	1
Caelo	Quinolina amarela	12051810	1
Caelo	Quinolina amarela	13109102	2
Caelo	Quinolina amarela	13109109	1
Caelo	Quinolina amarela	14049401	2
Caelo	Quinolina amarela	14274305	1
Caelo	Quinolina amarela	14274309	1
Caelo	Quinolina amarela	14363202	4
Caelo	Quinolina amarela	14363207	1
Caelo	Quinolina amarela	15276801	2
Caelo	Quinolina amarela	15276802	1
Caelo	Quinolina amarela	15276803	2
Caelo	Quinolina amarela	15276804	2
Caelo	Quinolina amarela	16050101	8
Caelo	Quinolina amarela	16050106	4
Caelo	Quinolina amarela	16050108	2
Caelo	Quinolina amarela	17034101	4
Caelo	Quinolina amarela	17034102	7
Caelo	Quinolina amarela	17034104	7
Caelo	Quinolina amarela	172277003	1
Caelo	Quinolina amarela	17227701	9
Caelo	Quinolina amarela	17227702	1
Caelo	Quinolina amarela	17227703	7
Caelo	Quinolina amarela	17227705	1
Caelo	Quinolina amarela	17227706	9
Caelo	Quinolina amarela	17227708	1
Caelo	Quinolina amarela	17227709	4
Caelo	Quinolina amarela	190734001	1
Caelo	Quinolina amarela	190734002	5
Caelo	Quinolina amarela	190734003	10
Caelo	Quinolina amarela	190734004	4
Caelo	Quinolina amarela	19073401	12
Caelo	Quinolina amarela	20002519003	1
Caelo	Quinolina amarela	20002519004	1
Caelo	Quinolina amarela	20002519005	3
Caelo	Quinolina amarela	20002519006	2
Caelo	Quinolina amarela	20301211-6	1
Caelo	Quinolina amarela	713E-03146	1
Caesar & Loretz GmbH...	Quinolina amarela	20002519012	1
Caesar & Loretz GmbH...	Quinolina amarela	20002519003	1
Caesar & Loretz GmbH	Quinolina amarela	17227705	1
Caesar & Loretz GmbH	Quinolina amarela	190734001	4
Caesar & Loretz GmbH	Quinolina amarela	190734002	1
Caesar & Loretz GmbH	Quinolina amarela	190734003	1
Caesar & Loretz GmbH	Quinolina amarela	190734004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Quinolina amarela	19073401	2
Caesar & Loretz GmbH	Quinolina amarela	20002519003	1
Caesar & Loretz GmbH	Quinolina amarela	20002519004	2
Caesar & Loretz GmbH	Quinolina amarela	20002519005	2
Caesar & Loretz GmbH	Quinolina amarela	20002519007	1
Caesar & Loretz GmbH	Quinolina amarela	20002519008	2
Caesar & Loretz GmbH	Quinolina amarela	20002519009	1
Caesar & Loretz GmbH	Quinolina amarela	2002519006	1
Fagron	Quinolina amarela	100427	1
Fagron	Quinolina amarela	11F30-N04	1
Fagron	Quinolina amarela	11K08-N01	2
Fagron	Quinolina amarela	12B08-N08	1
Fagron	Quinolina amarela	12E24-N05	1
Fagron	Quinolina amarela	12L11-N07	1
Fagron	Quinolina amarela	14D18-B02-295783	1
Fagron	Quinolina amarela	17227705	1
Fagron	Quinolina amarela	9878	1
Klosterring	Quinolina amarela	17227706	1
Noweda	Quinolina amarela	17227706	1
PHOENIX	Quinolina amarela	12042004	1
Phoenix	Quinolina amarela	20002519003	1
phönix	Quinolina amarela	15276803	1
Phönix	Quinolina amarela	16050108	1
sanacorp	Quinolina amarela	3214M-03146	1

- 235 888 spectra from 1515 *Apo-Ident* customers from a total of 49 198 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Quinolina amarela* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinolina amarela* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	220	0	201 864
Type C	0	179	0	235 888

The substance/substance group *Quinolina amarela* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.6480 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20922	21305	17,46	141,55
21305	21305	0,00	136,85
23400	23400	0,00	149,31
23685	23685	0,00	145,31
24812	24812	0,00	138,66
26737	26737	0,00	129,23
26962	26962	0,00	147,42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Resorcinol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20938-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Resorcinol; Resorcinolum

Special notes

When selecting the *Resorcinol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Resorcinol	9	5	103

Second-stage model

For differentiation of the substance/substance group *Resorcinol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Resorcinol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hidroquinona	37,32	–
Cromoglicato de sódio	97,96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Resorcinol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Resorcinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Resorcinol	13293108	21471	60	AR-15-FG-006906-01
Caelo	Resorcinol	161533	22632	40	20160524*
Caelo	Resorcinol	182166	25196	40	20181114*
Caelo	Resorcinol	22002981	26504	40	20221014*
Caelo	Resorcinol	22002981	26504SI	20	20221014*
Caelo	Resorcinol	23001796	26969	40	20230814*
Caelo	Resorcinol	23001796	26969SI	20	20230814*
Caelo	Resorcinol	24000513	27136	40	20240226*
Fagron	Resorcinol	12G24-N04	20938	40	1401462
Fagron	Resorcinol	13I18-B09-291533	21706	40	20130606
Fagron	Resorcinol	19J21-B16-195450	25171	40	20191105

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 11 reference samples from the substance/substance group *Resorcinol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 225 spectra of 7 reference samples from the substance/substance group *Resorcinol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Resorcinol	20003735	25736	50
Caelo	Resorcinol	21004158	26005	40
Caelo	Resorcinol	23003284	27117	40
Fagron	Resorcinol	17H03-B11-338899	23921	40
Fagron	Resorcinol	21F14-B01-213197	27240	40
Caelo	Resorcinol	21004158	26005SI	10
Fagron	Resorcinol	13I18-B09-291533	21706†	5

- 201 859 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 246 spectra from 167 *Apo-Ident* customers from 108 batches from the substance/substance group *Resorcinol*.

- Among them are spectra of independent samples from 103 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Resorcinol	21004158004	1
	Resorcinol	21004158008	2
	Resorcinol	21F14-B01-213197	1
	Resorcinol	22002981004	2
	Resorcinol	90972	1
Anzag	Resorcinol	18216615	1
Caelo	Resorcinol	10111210	1
Caelo	Resorcinol	10218809	2
Caelo	Resorcinol	11309610	4
Caelo	Resorcinol	11d29-n14	2
Caelo	Resorcinol	12255614	2
Caelo	Resorcinol	12G24-N04	2
Caelo	Resorcinol	13/18-B19-291534	1
Caelo	Resorcinol	13293103	1
Caelo	Resorcinol	13293110	1
Caelo	Resorcinol	13293115	2
Caelo	Resorcinol	15009502	1
Caelo	Resorcinol	15009507	8
Caelo	Resorcinol	15009511	4
Caelo	Resorcinol	15009515	2
Caelo	Resorcinol	15K24-B02-317584	1
Caelo	Resorcinol	16/13082	1
Caelo	Resorcinol	16153306	1
Caelo	Resorcinol	16153307	1
Caelo	Resorcinol	16153309	8
Caelo	Resorcinol	16153312	1
Caelo	Resorcinol	16153313	5
Caelo	Resorcinol	16271807	1
Caelo	Resorcinol	16D29-B01	1
Caelo	Resorcinol	18015601	1
Caelo	Resorcinol	18015603	1
Caelo	Resorcinol	18111703	1
Caelo	Resorcinol	18130901	3
Caelo	Resorcinol	182166002	1
Caelo	Resorcinol	18216601	1
Caelo	Resorcinol	18216603	7
Caelo	Resorcinol	18216607	2
Caelo	Resorcinol	18216609	1
Caelo	Resorcinol	18216610	1
Caelo	Resorcinol	18216611	7
Caelo	Resorcinol	18216615	1
Caelo	Resorcinol	18B08-B05-347787	3
Caelo	Resorcinol	19061305	1
Caelo	Resorcinol	19J21-16-I95450	1
Caelo	Resorcinol	20003735002	2
Caelo	Resorcinol	20003735007	3
Caelo	Resorcinol	2003735006	1
Caelo	Resorcinol	2041512	1
Caelo	Resorcinol	206370-0003	1
Caelo	Resorcinol	21004158004	2
Caelo	Resorcinol	24092001	1
Caelo	Resorcinol	5052	1
Caesar & Loretz GmbH...	Resorcinol	18216603	1
Caesar & Loretz GmbH/Gehe	Resorcinol	182166002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/L30	Resorcinol	21000873008	1
Caesar & Loretz GmbH...	Resorcinol	20003735007	1
Caesar & Loretz GmbH...	Resorcinol	18216601	1
Caesar & Loretz GmbH	Resorcinol	18216607	1
Caesar & Loretz GmbH	Resorcinol	18216609	1
Caesar & Loretz GmbH	Resorcinol	18216611	1
Caesar & Loretz GmbH	Resorcinol	18216613	1
Caesar & Loretz GmbH	Resorcinol	20003735005	2
Caesar & Loretz GmbH	Resorcinol	20003735006	2
Caesar & Loretz GmbH	Resorcinol	20003735007	1
Euro OTC	Resorcinol	11/13-N02	1
Euro OTC	Resorcinol	16D29-B01-329760	1
Fagron	Resorcinol	10B01-N06	2
Fagron	Resorcinol	11/13-N02	2
Fagron	Resorcinol	11/13-no2	1
Fagron	Resorcinol	1112013A	1
Fagron	Resorcinol	118b09291534	1
Fagron	Resorcinol	11A19-N09	1
Fagron	Resorcinol	11D29-N14	1
Fagron	Resorcinol	11L19-N19	2
Fagron	Resorcinol	12G24-N004	1
Fagron	Resorcinol	12g24-N04	1
Fagron	Resorcinol	12G24-N04	9
Fagron	Resorcinol	12K30-N03	4
Fagron	Resorcinol	13/17071	1
Fagron	Resorcinol	13/18-B09-291534	1
Fagron	Resorcinol	13E24-N10	8
Fagron	Resorcinol	13I18-B09	2
Fagron	Resorcinol	13I18-B09-291533	1
Fagron	Resorcinol	13I18-B09-291534	1
Fagron	Resorcinol	14/15-B02-307749	1
Fagron	Resorcinol	14/16062	1
Fagron	Resorcinol	14/19050	1
Fagron	Resorcinol	1415B02307749	1
Fagron	Resorcinol	14G10B06	1
Fagron	Resorcinol	14G10-B06-296296	7
Fagron	Resorcinol	14G10-B06-296297	2
Fagron	Resorcinol	14J15-B02	2
Fagron	Resorcinol	14J15-B02-307749	5
Fagron	Resorcinol	15/18082	1
Fagron	Resorcinol	15K24-B02-317584	3
Fagron	Resorcinol	1613082	1
Fagron	Resorcinol	16D29-B01	1
Fagron	Resorcinol	16d29b01323046	1
Fagron	Resorcinol	16D29-B01-323046	5
Fagron	Resorcinol	16D29-B01-329760	3
Fagron	Resorcinol	16d29b01332738	1
Fagron	Resorcinol	16D29-B01-332738	2
Fagron	Resorcinol	17H03-B11-338899	3
Fagron	Resorcinol	17H03-B11-342399	1
Fagron	Resorcinol	18/19081	1
Fagron	Resorcinol	18B08-B05-347787	5
Fagron	Resorcinol	18K20-B01-355679	1
Fagron	Resorcinol	19J21-B16195450	1
Fagron	Resorcinol	19J21-B16-195450	1
Fagron	Resorcinol	20E07-B09-200551	2
Fagron	Resorcinol	20129-B13	1
Fagron	Resorcinol	20L29-B13	2
Fagron	Resorcinol	20L29-B13-204180	6
Fagron	Resorcinol	211217(20L29-B13-204180)	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Resorcinol	2112I-02170	1
Fagron	Resorcinol	88735	1
Fagron	Resorcinol	B09-2005501	1
Fagron	Resorcinol	B16-1954500	1
Fargon/ Phönix	Resorcinol	16D29-B01-323046	1
Fargon	Resorcinol	15K24-B02-317584	1
Gehe	Resorcinol	11L13-N02	1
Gehe	Resorcinol	13E24-N10	1
L12	Resorcinol	16153306	1
Noweda/Fargon	Resorcinol	16029-B01-329760	1
Noweda	Resorcinol	1318b09291533	1
Noweda	Resorcinol	13E24-N10	1
Noweda	Resorcinol	14G10-B06-296	1
Noweda	Resorcinol	2003735007	1
Noweda	Resorcinol	21004158004	1
Phoenix WE: 13.07.2015	Resorcinol	14G10-B06-296296	1
Phoenix goettin	Resorcinol	13I18-B09-291534	1
Phönix Gotha	Resorcinol	14G10-B06-296296	1
Phönix	Resorcinol	20L29-B13	1
Sanacorp	Resorcinol	16D29-Bo1-323046	1
vdl	Resorcinol	12G24-N04	1

- 235 821 spectra from 1515 *Apo-Ident* customers from a total of 49 151 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Resorcinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Resorcinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	225	0	201 859
Type C	0	245	1	235 821

The substance/substance group *Resorcinol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.3333 %)
Type C	100.0000 % (> 99.9007 %)	99.5935 % (> 98.3740 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20938	20938	0,00	49,80
21471	21471	0,00	45,15
21706	21471	7,64	41,09
22632	22632	0,00	44,61
25171	21471	11,27	40,74
25196	25196	0,00	43,77
26504	26504	0,00	41,39
26969	26969	0,00	56,15
27136	27136	0,00	44,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Riboflavina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20409-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Riboflavina; Riboflavinum

Special notes

When selecting the *Riboflavina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Riboflavina	12	13	64

Second-stage model

For differentiation of the substance/substance group *Riboflavina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Riboflavina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	32,70	11,00
Fosfato sódico de riboflavina hidratado	32,95	–
Cromoglicato de sódio	69,24	–
⋮	⋮	⋮
Bacitracina	>50	30,58
Sulfato de colistina	>50	31,64
Anfotericina B	>50	44,66
Cianocobalamina	>50	55,10
Pantotenato de cálcio	>50	57,25
Nistatina	>50	57,71
Triancinolona	>50	62,49
Tosilcloramida sódica	>50	64,32
Glicerofosfato de cálcio	>50	76,30
Estradiol hemi-hidratado	>50	76,82
Bromidrato de hioscina	>50	79,63
Vitamina E acetato pó 50%	>50	100,70
SyrSpend® SF pH4 neo	>50	101,74
Levedura de selênio	>50	104,42
Estriol	>50	115,13
Metilcobalamina	>50	118,32
Gelatina, branca	>50	124,32
Carmelose sódica	>50	156,01
SyrSpend® SF Alka	>50	157,36
Amido de arroz	>50	164,48
Ácido oxálico	>50	198,69
SyrSpend® SF pH4	>50	252,66
Amido de milho	>50	268,93
Amido de trigo	>50	282,41
Goma arábica, dispersão seca	>50	307,30
Fécula de batata	>50	312,39
Frutose	>50	318,91
Maltodextrina	>50	350,99

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Riboflavina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Riboflavina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Riboflavina	12003317	20925	40	1405155
Caelo	Riboflavina	13305203	21389	60	AR-15-FG-005686-01
Caelo	Riboflavina	14322008	22492	40	AR-16-FG-013669-01
Caelo	Riboflavina	21000916	25654	40	20210408*
Euro OTC	Riboflavina	1701050	23004	40	20170214*
Euro OTC	Riboflavina	1701050-01	23091	40	20170214
Euro OTC	Riboflavina	2002026	25157	40	20200512*
Euro OTC	Riboflavina	2102005	25600	40	20210330*
Fagron	Riboflavina	13D02-N03	20825	40	AR-15-FG-000733-01
Fagron	Riboflavina	13D02-N03	20914	40	20130405
Fagron	Riboflavina	15G20-B13-310997	21955	60	20150819
Fagron	Riboflavina	16B18-B06-319026	22655	40	AR-16-FG-014466-01
Fagron	Riboflavina	17G14-B05-337885	23714	40	AR-18-FG-000141-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 560 spectra of 13 reference samples from the substance/substance group *Riboflavina*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.
- 152 402 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 600 spectra of 17 reference samples from the substance/substance group *Riboflavina*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Riboflavina	15330708	23579	40
Caelo	Riboflavina	172722	23649	40
Caelo	Riboflavina	192609	24884	40
Caelo	Riboflavina	22003300	26473	40
Caelo	Riboflavina	23003154	27129	40
Euro OTC	Riboflavina	1707017	23612	40
Euro OTC	Riboflavina	1801018	23880	40
Euro OTC	Riboflavina	1809004	24297	40
Euro OTC	Riboflavina	1810005	24307	40
Euro OTC	Riboflavina	2009015	25423	40
Euro OTC	Riboflavina	2210022	26437	40
Euro OTC	Riboflavina	2408013	27401	40
Fagron	Riboflavina	22D13-B02-219504	26398	40
Caelo	Riboflavina	22003300	26473SI	20
Caelo	Riboflavina	23003154	27129SI	20
Euro OTC	Riboflavina	2408013	27401SI	20
Fagron	Riboflavina	22D13-B02-219504	26398SI	20

- 201 484 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 111 spectra from 47 *Apo-Ident* customers from 69 batches from the substance/substance group *Riboflavina*.

- Among them are spectra of independent samples from 64 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Riboflavina	20004481001	1
	Riboflavina	22003300001	1
Anzag/Anzag 11.09.18	Riboflavina	18B22-B01-347142	1
Caelo	Riboflavina	15330708	2
Caelo	Riboflavina	17272204	2
Caelo	Riboflavina	17G14-B05-337885	1
Caelo	Riboflavina	21000916002	2
Caelo	Riboflavina	21000916003	1
Caelo	Riboflavina	21000916007	1
Caesar & Loretz GmbH...	Riboflavina	19000560002	1
Caesar & Loretz GmbH...	Riboflavina	18123401	1
Caesar & Loretz GmbH	Riboflavina	19000560002	1
Caesar & Loretz GmbH	Riboflavina	21000916002	1
EuRho	Riboflavina	1810005-01	1
Euro OTC	Riboflavina	1701050-02	1
Euro OTC	Riboflavina	1707017-01	1
Euro OTC	Riboflavina	19G17-B07	1
Euro OTC	Riboflavina	2102005-02	1
Euro OTC	Riboflavina	L1210048-01	1
Euro OTC	Riboflavina	L1305039-01	1
Fagr9n 06.11.19	Riboflavina	19F10B07191754	1
Fagron	Riboflavina	11K02-N01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Riboflavina	13J29-B04-287533	1
Fagron	Riboflavina	13J29-B04-287534	1
Fagron	Riboflavina	14B03B07292071	1
Fagron	Riboflavina	14E01-B10-296718	2
Fagron	Riboflavina	14K03-B04-304718	1
Fagron	Riboflavina	15G20-B13-310997	2
Fagron	Riboflavina	15I09-B02-315216	1
Fagron	Riboflavina	167720-0005	2
Fagron	Riboflavina	16B18_b06_319026	1
Fagron	Riboflavina	16B18-B06-321484	1
Fagron	Riboflavina	16E18-B05-325274	1
Fagron	Riboflavina	16E-18-B05-325274	1
Fagron	Riboflavina	16I12-B05-329618	1
Fagron	Riboflavina	16J12-B05-329618	2
Fagron	Riboflavina	1701050-01	1
Fagron	Riboflavina	17G14-B05-337885	1
Fagron	Riboflavina	17H10-B06-340170	3
Fagron	Riboflavina	18822-B01-347142	2
Fagron	Riboflavina	18D05-B04	1
Fagron	Riboflavina	18D05B04349962	1
Fagron	Riboflavina	18J10-B01	2
Fagron	Riboflavina	18J10-B01-355004	4
Fagron	Riboflavina	18J10-B01-356142	1
Fagron	Riboflavina	19F10-B07-191754	4
Fagron	Riboflavina	19F-10-B07-191754	1
Fagron	Riboflavina	19g17-b07-192788	1
Fagron	Riboflavina	19G17-B07-192788	5
Fagron	Riboflavina	19G17-B07-200577	5
Fagron	Riboflavina	19GT-B07-192788	2
Fagron	Riboflavina	20a14-b04-196790	1
Fagron	Riboflavina	20A14-B04-196790	1
Fagron	Riboflavina	20A14-BO4-196790	1
Fagron	Riboflavina	21A14-B03-210578	6
Fagron	Riboflavina	21D07-B10-218559	3
Fagron	Riboflavina	22B26-B01	1
Fagron	Riboflavina	22D13-B02	3
Fagron	Riboflavina	22D13-B02-219504	3
Fagron	Riboflavina	22L13-B16-226589	1
Fagron	Riboflavina	BO4-1967900	1
Fagron	Riboflavina	BO4-1967900	1
Fagron	Riboflavina	BO7-2005707	1
Fagron	Riboflavina	RIB3061HF	2
Fagron	Riboflavina	UQ00510683	1
Fagron	Riboflavina	UQ60910194	1
Fagron	Riboflavina	UQ70210050	1
Fagron	Riboflavina	UQ80810145	1
Fagron	Riboflavina	UQ90410074	1
Gatt-Koller	Riboflavina	1803007	1
Noweda	Riboflavina	18J10-B01-355004	1
Noweda	Riboflavina	19F01-B07-191754	1
Vdl 09.05.14;Preis 7,45	Riboflavina	13305203/15R05	1

- 235 956 spectra from 1515 *Apo-Ident* customers from a total of 49 189 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Riboflavina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Riboflavina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	560	0	152 402
Type B	0	600	0	201 484
Type C	0	110	1	235 956

The substance/substance group *Riboflavina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9286 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.0991 % (> 96.3964 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20825	20825	0,00	85,48
20914	20825	15,04	85,53
20925	20925	0,00	92,48
21389	21389	0,00	93,13
21955	21389	12,70	96,06
22492	22492	0,00	101,26
22655	22655	0,00	98,91
23004	23004	0,00	90,90
23091	23714	19,20	93,75
23714	23714	0,00	96,81
25157	25157	0,00	91,43
25600	25600	0,00	111,95
25654	25654	0,00	101,63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sacarina sódica**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20200-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sacarina sódica; Saccharinum natricum

Special notes

When selecting the *Sacarina sódica* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sacarina sódica	10	6	76

Second-stage model

For differentiation of the substance/substance group *Sacarina sódica* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sacarina sódica* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Quinolina amarela	83,75	24,00
⋮	⋮	⋮
Furoato de mometasona	>50	100,04
Sulfato de atropina	>50	109,35
Escina, hidrossolúvel	>50	123,96
Cloridrato de propranolol	>50	163,58
Citrato monobásico de magnésio, hid…	>50	204,36
Hidrocortisona	>50	224,98
Fenitoína	>50	250,77
Orotato de cálcio di-hidratado	>50	299,96
Sorbato de potássio	>50	422,23

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sacarina sódica* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sacarina sódica*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sacarina sódica	172110	23643	40	20170831*
Caelo	Sacarina sódica	162210	23857	39	20160811*
Caelo	Sacarina sódica	172592	24409	40	20171206*
Caelo	Sacarina sódica	19000658	25214	40	20200121*
Caelo	Sacarina sódica	21003326	26008	40	20220105*
Caelo	Sacarina sódica	23003299	27121	40	20240124*
Fagron	Sacarina sódica	13I20-B06-291654	23020	40	AR-17-FG-012457-01
Fagron	Sacarina sódica	14F30-B02-296322	23452	40	AR-17-FG-022421-01
Fagron	Sacarina sódica	14F30-B02-296322	23453	40	AR-18-FG-007117-02
Fagron	Sacarina sódica	18L06-B01-361488	25178	40	20190130
Fagron	Sacarina sódica	22K28-B09-221810	26615	40	20230112
Fagron	Sacarina sódica	22K28-B09-221810	26615SI	20	20230112

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 459 spectra of 12 reference samples from the substance/substance group *Sacarina sódica*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 503 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Sacarina sódica*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sacarina sódica	15087704	22769	40
Caelo	Sacarina sódica	182104	24381	40
Caelo	Sacarina sódica	190964	24499	40
Caelo	Sacarina sódica	22003584	26489	40
Caelo	Sacarina sódica	23000898	26701	40
Caelo	Sacarina sódica	24001228	27251	40
Caelo	Sacarina sódica	21003326	26008SI†	10
Caelo	Sacarina sódica	22003584	26489SI	20

- 201 814 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 435 spectra from 323 *Apo-Ident* customers from 79 batches from the substance/substance group *Sacarina sódica*.
- Among them are spectra of independent samples from 76 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sacarina sódica		1
	Sacarina sódica	21003326011	1
	Sacarina sódica	21003326015	3
	Sacarina sódica	21003326024	5
	Sacarina sódica	2200354008	1
	Sacarina sódica	22003558008	1
	Sacarina sódica	22003584008	1
	Sacarina sódica	22003584014	2
	Sacarina sódica	23000898005	1
17270001	Sacarina sódica	17211002	1
Alliance Healtcare	Sacarina sódica	20004198009	1
Cael Sanacorp 05.02.2016	Sacarina sódica	15087703	1
Caeleo/ Krieger	Sacarina sódica	17329407	1
Caelo	Sacarina sódica		1
Caelo	Sacarina sódica	11025605	1
Caelo	Sacarina sódica	11025610	1
Caelo	Sacarina sódica	11172805	3
Caelo	Sacarina sódica	11172814	1
Caelo	Sacarina sódica	12139803	1
Caelo	Sacarina sódica	1236207	1
Caelo	Sacarina sódica	12362607	3
Caelo	Sacarina sódica	13205411	1
Caelo	Sacarina sódica	13205414	3
Caelo	Sacarina sódica	13205417	1
Caelo	Sacarina sódica	1402970	1
Caelo	Sacarina sódica	14029705	6
Caelo	Sacarina sódica	14029707	3
Caelo	Sacarina sódica	14029709	1
Caelo	Sacarina sódica	14029710	3
Caelo	Sacarina sódica	14213402	3
Caelo	Sacarina sódica	14213405	5
Caelo	Sacarina sódica	15084101	6
Caelo	Sacarina sódica	15087703	7
Caelo	Sacarina sódica	15087704	12
Caelo	Sacarina sódica	15087707	3
Caelo	Sacarina sódica	15087713	18
Caelo	Sacarina sódica	16221005	14
Caelo	Sacarina sódica	16221009	4
Caelo	Sacarina sódica	16221010	1
Caelo	Sacarina sódica	17211001	2
Caelo	Sacarina sódica	17211002	18
Caelo	Sacarina sódica	17211002P-190808-4	1
Caelo	Sacarina sódica	17211005	2
Caelo	Sacarina sódica	17329309	1
Caelo	Sacarina sódica	17329310	10
Caelo	Sacarina sódica	17329405	4
Caelo	Sacarina sódica	17329407	11

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sacarina sódica	17329409	17
Caelo	Sacarina sódica	18210407	13
Caelo	Sacarina sódica	19000658002	12
Caelo	Sacarina sódica	19000658005	5
Caelo	Sacarina sódica	1906403	1
Caelo	Sacarina sódica	190964001	8
Caelo	Sacarina sódica	19096403	17
Caelo	Sacarina sódica	19096408	1
Caelo	Sacarina sódica	20000953001	13
Caelo	Sacarina sódica	20000953003	2
Caelo	Sacarina sódica	20000953006	6
Caelo	Sacarina sódica	20004198004	3
Caelo	Sacarina sódica	20004198005	8
Caelo	Sacarina sódica	20004198009	15
Caelo	Sacarina sódica	21003326006	6
Caelo	Sacarina sódica	21003326007	1
Caelo	Sacarina sódica	21003326011	5
Caelo	Sacarina sódica	21003326015	1
Caelo	Sacarina sódica	21003326019	6
Caelo	Sacarina sódica	21003326024	1
Caelo	Sacarina sódica	21092015A	1
Caelo	Sacarina sódica	220905(21003326011)	1
Caelo	Sacarina sódica	3414M-02206	1
Caelo	Sacarina sódica	3518E-02206	1
Caelo	Sacarina sódica	8121801	1
Caelo	Sacarina sódica	90542309	1
Caelo	Sacarina sódica	9381714	1
Caelo	Sacarina sódica	B190964001	1
Caesar & Loretz GmbH…	Sacarina sódica	21003326011	2
Caesar & Loretz GmbH…	Sacarina sódica	21003326015	3
Caesar & Loretz GmbH…	Sacarina sódica	21003326019	4
Caesar & Loretz GmbH…	Sacarina sódica	17329407	1
Caesar & Loretz GmbH…	Sacarina sódica	13205418	2
Caesar & Loretz GmbH…	Sacarina sódica	20004198005	1
Caesar & Loretz GmbH/AHD	Sacarina sódica	20004198005	1
Caesar & Loretz GmbH/AHD	Sacarina sódica	21003326019	1
Caesar & Loretz GmbH…	Sacarina sódica	20000953001	1
Caesar & Loretz GmbH/E	Sacarina sódica	21003326011	1
Caesar & Loretz GmbH/Gehe	Sacarina sódica	20000953	1
Caesar & Loretz GmbH…	Sacarina sódica	21003326006	1
Caesar & Loretz GmbH…	Sacarina sódica	21003326006	1
Caesar & Loretz GmbH…	Sacarina sódica	21003326024	1
Caesar & Loretz GmbH…	Sacarina sódica	19096403	2
Caesar & Loretz GmbH/Sa	Sacarina sódica	20004198004	1
Caesar & Loretz GmbH…	Sacarina sódica	20004198004	1
Caesar & Loretz GmbH…	Sacarina sódica	20004198006	1
Caesar & Loretz GmbH	Sacarina sódica	17211002	1
Caesar & Loretz GmbH	Sacarina sódica	17329310	2
Caesar & Loretz GmbH	Sacarina sódica	17329311	1
Caesar & Loretz GmbH	Sacarina sódica	17329409	1
Caesar & Loretz GmbH	Sacarina sódica	18210407	4
Caesar & Loretz GmbH	Sacarina sódica	19000658002	1
Caesar & Loretz GmbH	Sacarina sódica	190964001	3
Caesar & Loretz GmbH	Sacarina sódica	19096403	4
Caesar & Loretz GmbH	Sacarina sódica	20000953001	6
Caesar & Loretz GmbH	Sacarina sódica	20004198004	1
Caesar & Loretz GmbH	Sacarina sódica	20004198005	5
Caesar & Loretz GmbH	Sacarina sódica	20004198009	7
Caesar & Loretz GmbH	Sacarina sódica	21003326006	5
Caesar & Loretz GmbH	Sacarina sódica	21003326011	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sacarina sódica	21003326015	1
Caesar & Loretz GmbH	Sacarina sódica	21003326019	2
Caesar & Loretz Hild…	Sacarina sódica	190964001	1
Caesar & Loretz Hilden	Sacarina sódica	17329407	1
Caesar & Loretz/Geil…	Sacarina sódica	20000953001	1
Caesar Loretz	Sacarina sódica	20000953001	1
Caesar&Lorenz	Sacarina sódica	19000658005	1
Caesar&loretz,Phoenix	Sacarina sódica	15084101	1
Cealo/ Noweda	Sacarina sódica	17329407	1
cealo	Sacarina sódica	15087703	1
Cealo	Sacarina sódica	17329405	1
Cealo	Sacarina sódica	19000658002	1
Euro OTC	Sacarina sódica	15087704	1
Euro OTC	Sacarina sódica	15087713	1
Fagron	Sacarina sódica	12A13-N03	2
Fagron	Sacarina sódica	12K26-N09	1
Fagron	Sacarina sódica	13D19-N01	1
Fagron	Sacarina sódica	SH349/12	1
Fargon	Sacarina sódica	12A13-N03	1
Gehe	Sacarina sódica	18210407	2
Gehe	Sacarina sódica	21003326011	1
Gehe	Sacarina sódica	23003240002	1
Henry Lamotte/AHD	Sacarina sódica	17329405	1
Ichthyol-Gesellschaft	Sacarina sódica	16221009	1
Jenne	Sacarina sódica	15087707	1
Jenne	Sacarina sódica	22003584008	1
Kehr	Sacarina sódica	17329407	1
Nachprüfung von Nove…	Sacarina sódica	14029707	2
Noweda	Sacarina sódica	20000953001	1
Noweda	Sacarina sódica	20000953003	1
Noweda	Sacarina sódica	21003326024	1
Pharmachem	Sacarina sódica	17329407	1
Phoenix	Sacarina sódica	14F30-B02-296322	1
Phönix	Sacarina sódica	17329407	1
Phönix	Sacarina sódica	19000658002	1
Phönix	Sacarina sódica	22003584014	1
Sana 03.11.14 EK 3,95	Sacarina sódica	14029707	1
sanacorp	Sacarina sódica	13205418	1
Sanacorp	Sacarina sódica	17211002	2

- 235 632 spectra from 1515 *Apo-Ident* customers from a total of 49 180 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sacarina sódica* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sacarina sódica* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	459	0	152 503
Type B	0	270	0	201 814
Type C	0	435	0	235 632

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Sacarina sódica* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6928 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6207 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23020	23020	0,00	178,29
23452	23452	0,00	190,79
23453	23453	0,00	192,50
23643	23643	0,00	218,53
23857	23857	0,00	218,78
24409	24409	0,00	217,04
25178	23857	30,06	213,85
25214	25214	0,00	143,70
26008	26008	0,00	155,90
26615	23643	25,30	220,54
27121	27121	0,00	189,31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sacarose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20372-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sacarose; Saccharum

Special notes

When selecting the *Sacarose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sacarose	13	8	696

Second-stage model

For differentiation of the substance/substance group *Sacarose* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sacarose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	57,03	–
⋮	⋮	⋮
Citrato de sódio	>50	76,51
Heparina sódica	>50	122,97
Capsaicina	>50	255,90
Amifampridina	>50	421,29
Cloridrato de quinina di-hidratado	>50	459,42
Cloridrato de oxibutinina	>50	515,33
Levocarnitina	>50	554,22
Prednicarbato	>50	618,68
Piridoxal-5-fosfato	>50	661,74
Cloridrato de ciprofloxacina	>50	836,42
Metoxisaleno	>50	910,90
Triclosan	>50	917,45
Alfaestradiol	>50	967,42
Tetracaína	>50	1084,88
Acetato de ciproterona	>50	1479,83
Acetato de noretisterona	>50	1574,56
Cloridrato de amitriptilina	>50	2918,29
Valina	>50	3858,21

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sacarose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sacarose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sacarose	13352909	21484	40	1410501
Caelo	Sacarose	14340003	21736	60	20141114

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sacarose	161999	22615	40	20160714*
Caelo	Sacarose	162060	22643	40	20160808*
Caelo	Sacarose	163286	23057	40	20161219*
Caelo	Sacarose	163081	23058	40	20161115*
Caelo	Sacarose	171066	23297	40	20170511*
Caelo	Sacarose	172133	23666	40	20170817*
Caelo	Sacarose	173247	23833	40	20180117*
Caelo	Sacarose	181582	24217	40	20180605*
Caelo	Sacarose	21000656	25651	40	20210406*
Caelo	Sacarose	22002704	26630	40	20220909*
Caelo	Sacarose	22002704	26630SI	20	20220909*
Caelo	Sacarose	23000893	26723	40	20230601*
Caelo	Sacarose	23000893	26723SI	20	20230601*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 580 spectra of 15 reference samples from the substance/substance group *Sacarose*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.
- 152 382 spectra from a total of 2829 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 340 spectra of 9 reference samples from the substance/substance group *Sacarose*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sacarose	12146801	20909	40
Caelo	Sacarose	181546	24237	40
Caelo	Sacarose	182574	24353	40
Caelo	Sacarose	182818	24359	40
Caelo	Sacarose	192839	25235	40
Caelo	Sacarose	190627	25236	40
Caelo	Sacarose	24000032	27134	40
Caelo	Sacarose	24002338	27447	40
Caelo	Sacarose	24000032	27134SI	20

- 201 744 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1771 spectra from 483 *Apo-Ident* customers from 700 batches from the substance/substance group *Sacarose*.
- Among them are spectra of independent samples from 695 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sacarose	13352908	1
	Sacarose	21003804004	3
	Sacarose	21003804007	1
	Sacarose	21003804012	9
	Sacarose	22002704004	10
	Sacarose	22002704005	2
	Sacarose	2202704004	1
	Sacarose	222704004	1
	Sacarose	23000893002	6
	Sacarose	23003269004	3
AHD	Sacarose	15182805	1
AHD	Sacarose	18154602	1
AHD	Sacarose	18154603	2
Audor Pharma	Sacarose	16206102	1
Bombastus	Sacarose	15156008	1
Cael	Sacarose	15182804	3
Caelo	Sacarose		1
Caelo	Sacarose	1(192839004)	1
Caelo	Sacarose	11246306	1
Caelo	Sacarose	11246313	2
Caelo	Sacarose	12107805	1
Caelo	Sacarose	12107806	2
Caelo	Sacarose	12241801	1
Caelo	Sacarose	12241803	2
Caelo	Sacarose	12241804	2
Caelo	Sacarose	12241808	5
Caelo	Sacarose	12241817	2
Caelo	Sacarose	12280309	1
Caelo	Sacarose	130031417	1
Caelo	Sacarose	13031405	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sacarose	13031406	2
Caelo	Sacarose	13031409	1
Caelo	Sacarose	13031410	2
Caelo	Sacarose	13031414	1
Caelo	Sacarose	13031417	2
Caelo	Sacarose	13063907	1
Caelo	Sacarose	13111706	1
Caelo	Sacarose	13352901	2
Caelo	Sacarose	13352902	13
Caelo	Sacarose	13352905	1
Caelo	Sacarose	13352908	1
Caelo	Sacarose	13352909	4
Caelo	Sacarose	13352911	1
Caelo	Sacarose	13352916	3
Caelo	Sacarose	13352920	5
Caelo	Sacarose	1352920	1
Caelo	Sacarose	14197301	4
Caelo	Sacarose	14197302	3
Caelo	Sacarose	14197313	1
Caelo	Sacarose	1430009	1
Caelo	Sacarose	14340003	4
Caelo	Sacarose	14340004	5
Caelo	Sacarose	14340005	1
Caelo	Sacarose	14340006	1
Caelo	Sacarose	14340008	5
Caelo	Sacarose	14340009	4
Caelo	Sacarose	15028801	14
Caelo	Sacarose	15028802	7
Caelo	Sacarose	15156008	1
Caelo	Sacarose	15182804	25
Caelo	Sacarose	15182805	3
Caelo	Sacarose	154460	1
Caelo	Sacarose	15446002	11
Caelo	Sacarose	15446003	7
Caelo	Sacarose	15446007	1
Caelo	Sacarose	160499	1
Caelo	Sacarose	16049902	3
Caelo	Sacarose	16049907	17
Caelo	Sacarose	16051301	1
Caelo	Sacarose	16051304	1
Caelo	Sacarose	16051305	2
Caelo	Sacarose	16166003	1
Caelo	Sacarose	162061	1
Caelo	Sacarose	16206102	13
Caelo	Sacarose	16206103	6
Caelo	Sacarose	1628603	1
Caelo	Sacarose	16305501	1
Caelo	Sacarose	16325605	1
Caelo	Sacarose	16328603	12
Caelo	Sacarose	16328605	22
Caelo	Sacarose	16328606	7
Caelo	Sacarose	16328607	22
Caelo	Sacarose	16351702	1
Caelo	Sacarose	1649902	1
Caelo	Sacarose	17021620306	1
Caelo	Sacarose	17042103	4
Caelo	Sacarose	17106601	1
Caelo	Sacarose	17106603	57
Caelo	Sacarose	17106604	22
Caelo	Sacarose	17247203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sacarose	17288702	1
Caelo	Sacarose	17354506	20
Caelo	Sacarose	18024405	41
Caelo	Sacarose	18024407	4
Caelo	Sacarose	1802445	1
Caelo	Sacarose	18154602	15
Caelo	Sacarose	18154603	28
Caelo	Sacarose	18257401	16
Caelo	Sacarose	18257402	52
Caelo	Sacarose	18260801	1
Caelo	Sacarose	18281803	4
Caelo	Sacarose	18281804	23
Caelo	Sacarose	18281810	2
Caelo	Sacarose	18329702	29
Caelo	Sacarose	18329703	9
Caelo	Sacarose	19060320648	1
Caelo	Sacarose	19060320649	1
Caelo	Sacarose	19060320650	1
Caelo	Sacarose	190627001	3
Caelo	Sacarose	190627002	23
Caelo	Sacarose	19062701	43
Caelo	Sacarose	19062702	4
Caelo	Sacarose	19132301	2
Caelo	Sacarose	1928339004	1
Caelo	Sacarose	192839001	1
Caelo	Sacarose	192839002	5
Caelo	Sacarose	192839004	33
Caelo	Sacarose	192839006	4
Caelo	Sacarose	192839007	26
Caelo	Sacarose	1928839004	1
Caelo	Sacarose	2(192839007)	1
Caelo	Sacarose	20001028003	1
Caelo	Sacarose	20002000004	1
Caelo	Sacarose	20003141002	1
Caelo	Sacarose	20003432001	1
Caelo	Sacarose	20004028001	3
Caelo	Sacarose	20004028003	22
Caelo	Sacarose	20011401	1
Caelo	Sacarose	20031515	1
Caelo	Sacarose	2100065004	1
Caelo	Sacarose	2100065006	1
Caelo	Sacarose	2100065007	1
Caelo	Sacarose	210006560001	1
Caelo	Sacarose	21000656001	22
Caelo	Sacarose	21000656004	4
Caelo	Sacarose	21000656006	11
Caelo	Sacarose	21000656007	4
Caelo	Sacarose	21000656010	12
Caelo	Sacarose	21003804003	4
Caelo	Sacarose	21003804004	18
Caelo	Sacarose	21003804007	7
Caelo	Sacarose	21003804008	2
Caelo	Sacarose	21003804011	1
Caelo	Sacarose	21003804012	3
Caelo	Sacarose	21003804013	2
Caelo	Sacarose	2100380412	1
Caelo	Sacarose	21003B	1
Caelo	Sacarose	22002704004	1
Caelo	Sacarose	24061502	1
Caelo	Sacarose	27111802	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sacarose	28041504	1
Caelo	Sacarose	28081308	1
Caelo	Sacarose	29081502	1
Caelo	Sacarose	4028003	1
Caelo	Sacarose	8024405	1
Caelo	Sacarose	81172478	2
Caelo	Sacarose	8704717	1
Caelo	Sacarose	Caelo14197301	1
Caeol/ Sanacorp	Sacarose	21000656001	1
Caeol/Sanacorp	Sacarose	18154603	1
Caeolo/Gehe	Sacarose	15446002	1
Caeolo/NOWEDA	Sacarose	21003804008	1
Caesar & Loretz GmbH...	Sacarose	16049907	1
Caesar & Loretz GmbH...	Sacarose	192839006	2
Caesar & Loretz GmbH...	Sacarose	21000656007	1
Caesar & Loretz GmbH...	Sacarose	192839006	1
Caesar & Loretz GmbH...	Sacarose	192839007	1
Caesar & Loretz GmbH...	Sacarose	190627002	1
Caesar & Loretz GmbH...	Sacarose	20004028003	1
Caesar & Loretz GmbH...	Sacarose	20004028003	2
Caesar & Loretz GmbH...	Sacarose	21000656010	1
Caesar & Loretz GmbH/G	Sacarose	18257402	1
Caesar & Loretz GmbH/Gehe	Sacarose	192839007	1
Caesar & Loretz GmbH/Gehe	Sacarose	20004028003	1
Caesar & Loretz GmbH/Gehe	Sacarose	21003804004	1
Caesar & Loretz GmbH...	Sacarose	192839006	1
Caesar & Loretz GmbH...	Sacarose	21000656007	1
Caesar & Loretz GmbH...	Sacarose	18281804	2
Caesar & Loretz GmbH...	Sacarose	18329703	1
Caesar & Loretz GmbH...	Sacarose	192839004	1
Caesar & Loretz GmbH...	Sacarose	19062701	3
Caesar & Loretz GmbH...	Sacarose	21000656001	1
Caesar & Loretz GmbH...	Sacarose	21003804012	1
Caesar & Loretz GmbH/Sana	Sacarose	20004028001	1
Caesar & Loretz GmbH...	Sacarose	17354506	1
Caesar & Loretz GmbH...	Sacarose	190627002	1
Caesar & Loretz GmbH...	Sacarose	19062701	1
Caesar & Loretz GmbH...	Sacarose	192839007	1
Caesar & Loretz GmbH...	Sacarose	21000656001	1
Caesar & Loretz GmbH...	Sacarose	21000656006	1
Caesar & Loretz GmbH	Sacarose	16328605	1
Caesar & Loretz GmbH	Sacarose	18154601	1
Caesar & Loretz GmbH	Sacarose	18154603	1
Caesar & Loretz GmbH	Sacarose	18257401	4
Caesar & Loretz GmbH	Sacarose	18257402	7
Caesar & Loretz GmbH	Sacarose	18281803	1
Caesar & Loretz GmbH	Sacarose	18281804	8
Caesar & Loretz GmbH	Sacarose	18329702	10
Caesar & Loretz GmbH	Sacarose	18329703	2
Caesar & Loretz GmbH	Sacarose	190627001	2
Caesar & Loretz GmbH	Sacarose	190627002	8
Caesar & Loretz GmbH	Sacarose	19062701	8
Caesar & Loretz GmbH	Sacarose	19062706	1
Caesar & Loretz GmbH	Sacarose	192839001	3
Caesar & Loretz GmbH	Sacarose	192839002	5
Caesar & Loretz GmbH	Sacarose	192839004	7
Caesar & Loretz GmbH	Sacarose	192839006	2
Caesar & Loretz GmbH	Sacarose	192839007	13
Caesar & Loretz GmbH	Sacarose	20004028003	11
Caesar & Loretz GmbH	Sacarose	21000656001	14

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sacarose	21000656006	4
Caesar & Loretz GmbH	Sacarose	21000656007	1
Caesar & Loretz GmbH	Sacarose	21000656010	8
Caesar & Loretz GmbH	Sacarose	21003804004	4
Caesar & Loretz GmbH	Sacarose	21003804007	9
Caesar & Loretz GmbH	Sacarose	21003804012	1
Caesar & Loretz GmbH	Sacarose	21003804013	1
Caesar & Loretz Hilden	Sacarose	18257402	1
Caesar & Loretz/Noweda	Sacarose	18329702	1
Caesar und Loretz	Sacarose	18329702	1
Caleo/ Noweda	Sacarose	17106603	1
Calo, Hilden/ Phönix	Sacarose	190627002	1
Cealo	Sacarose	15446002	1
Cealo	Sacarose	16206102	1
DHU	Sacarose	7020407	1
DHU	Sacarose	9010709	1
DHU	Sacarose	9010710	1
DHU	Sacarose	9020110	1
DHU	Sacarose	9020510	1
DHU	Sacarose	9050610	1
Diamant	Sacarose	L24223	1
Euro OTC	Sacarose	12345	2
Euro OTC	Sacarose	16328605	1
Euro OTC	Sacarose	17106603	1
Euro OTC	Sacarose	17354506	1
Euro OTC	Sacarose	18024405	2
Fagron	Sacarose	1011208731	2
Fagron	Sacarose	11/16-N01	1
Fagron	Sacarose	11/16-NO1	1
Fagron	Sacarose	11/20-N05	1
Fagron	Sacarose	11E19-N04	1
Fagron	Sacarose	11I16-N01	1
Fagron	Sacarose	11L09-N16	2
Fagron	Sacarose	12-E03-M01	1
Fagron	Sacarose	12E29-N04	1
Fagron	Sacarose	12G26-N01	2
Fagron	Sacarose	13A07-N03	1
Fagron	Sacarose	13D29-N08	1
Fagron	Sacarose	13G03-N16	1
Fagron	Sacarose	13G04-N01	1
Fagron	Sacarose	13I30-N05	1
Fagron	Sacarose	15446002	1
Fagron	Sacarose	16206102	1
Fagron	Sacarose	18082014D	1
Fagron	Sacarose	18257402	1
Fagron	Sacarose	2102308731	1
Fagron	Sacarose	5071201	1
Fagron	Sacarose	5112I-02207	1
Fargon	Sacarose	19I30-T05-079071	1
Gehe Weiterstadt	Sacarose	21003804012	1
Gehe	Sacarose	1434006	1
Gehe	Sacarose	15028802	1
Gehe	Sacarose	15446003	2
Gehe	Sacarose	16328607	1
GEHE	Sacarose	16328607	1
Gehe	Sacarose	17106603	1
Gehe	Sacarose	18281804	1
Gehe	Sacarose	18329702	2
Gehe	Sacarose	192839007	1
Gehe	Sacarose	21000656001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Sacarose	21000656004	2
Hanns G.Werner GmbH	Sacarose	8731158	1
Haushalt	Sacarose	123456	1
Jenne	Sacarose	15182804	1
Jenne	Sacarose	18257402	2
Jenne	Sacarose	24000032005	1
Kaufland	Sacarose	L24475	1
Kaufland	Sacarose	L24494	2
Kehr	Sacarose	16328606	1
Kehr	Sacarose	190627002	1
L12	Sacarose	18154603	1
Lebensmittelware (Edeka)	Sacarose		1
Noweda	Sacarose	13352920	2
Noweda	Sacarose	16328603	1
Noweda	Sacarose	16328607	1
Noweda	Sacarose	18154603	1
Noweda	Sacarose	220002704004	1
Penny Markt	Sacarose	201L113530100	3
Penny Markt	Sacarose	L120325600	2
Penny Markt	Sacarose	L120404100	3
Penny Markt	Sacarose	L120612100	3
Penny Markt	Sacarose	L120628000	3
Penny	Sacarose	L12513800	3
Pfeifer/Langen	Sacarose	L03144N	1
Pharmachem	Sacarose	7878	1
pharm-a-speres	Sacarose	8731003	1
pharm-a-spheres/sana…	Sacarose	8731306	1
Phoenix	Sacarose	18257402	1
Phoenix	Sacarose	190627002	2
Phoenix	Sacarose	192839004	1
phoenix	Sacarose	2100656001	1
Phönix	Sacarose	15446002	1
phönix	Sacarose	16351701	1
PHÖNIX	Sacarose	17106603	1
Phönix	Sacarose	18154603	3
Phönix	Sacarose	192839004	2
ROHA	Sacarose	130090	1
Salvator Apotheke	Sacarose	R2229455M	1
Sanacorp/Caela	Sacarose	17106603	1
Sanacorp	Sacarose	14197301	1
Sanacorp	Sacarose	14340005	1
Sanacorp	Sacarose	17106603	1
Sanacorp	Sacarose	192839007	1
Sanacorp	Sacarose	22002704004	1
Sanacorp	Sacarose	23000893002	1
Sanacorp	Sacarose	AKD5	1
Soldan	Sacarose		1
Soldan	Sacarose	232027	1
Soldan	Sacarose	243983	1
Spagyra Österreich	Sacarose	15112321097	1
Spagyra Österreich	Sacarose	21102920359	1
Spagyra/Österreich	Sacarose	10070521044	1
Spagyra/Österreich	Sacarose	12112721050	1
Spagyra/Österreich	Sacarose	13021920149	1
Spagyra/Österreich	Sacarose	13050621774	1
Spagyra/Österreich	Sacarose	13091920456	1
Spagyra/Österreich	Sacarose	13102520353	1
Spagyra/Österreich	Sacarose	13111121193	1
Spagyra/Österreich	Sacarose	14010721509	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sacarose	14012420377	1
Spagyra/Österreich	Sacarose	14041421810	1
Spagyra/Österreich	Sacarose	14050621091	1
Spagyra/Österreich	Sacarose	14060353342	1
Spagyra/Österreich	Sacarose	14060353343	1
Spagyra/Österreich	Sacarose	14070721041	1
Spagyra/Österreich	Sacarose	14071421137	2
Spagyra/Österreich	Sacarose	16122820921	1
Spagyra/Österreich	Sacarose	1624	1
Spagyra/Österreich	Sacarose	17020820810	1
Spagyra/Österreich	Sacarose	17020820816	1
Spagyra/Österreich	Sacarose	17021620307	1
Spagyra/Österreich	Sacarose	17021620309	1
Spagyra/Österreich	Sacarose	17022022188	1
Spagyra/Österreich	Sacarose	17032120927	1
Spagyra/Österreich	Sacarose	17032321132	1
Spagyra/Österreich	Sacarose	17032820797	1
Spagyra/Österreich	Sacarose	17041821026	1
Spagyra/Österreich	Sacarose	17041821027	1
Spagyra/Österreich	Sacarose	17070320627	1
Spagyra/Österreich	Sacarose	17091520139	1
Spagyra/Österreich	Sacarose	17092620773	1
Spagyra/Österreich	Sacarose	17121420710	1
Spagyra/Österreich	Sacarose	1721420709	1
Spagyra/Österreich	Sacarose	18021921250	1
Spagyra/Österreich	Sacarose	18032320385	1
Spagyra/Österreich	Sacarose	18032320386	1
Spagyra/Österreich	Sacarose	18032320387	1
Spagyra/Österreich	Sacarose	18032320388	1
Spagyra/Österreich	Sacarose	18041120712	1
Spagyra/Österreich	Sacarose	18041180714	1
Spagyra/Österreich	Sacarose	18042720542	1
Spagyra/Österreich	Sacarose	18042720555	2
Spagyra/Österreich	Sacarose	18051421069	1
Spagyra/Österreich	Sacarose	18051421071	1
Spagyra/Österreich	Sacarose	18072420037	1
Spagyra/Österreich	Sacarose	18090520787	3
Spagyra/Österreich	Sacarose	18090520788	1
Spagyra/Österreich	Sacarose	18090520789	1
Spagyra/Österreich	Sacarose	18091020640	1
Spagyra/Österreich	Sacarose	18092720503	1
Spagyra/Österreich	Sacarose	1809272503	1
Spagyra/Österreich	Sacarose	18111921057	1
Spagyra/Österreich	Sacarose	18112920404	1
Spagyra/Österreich	Sacarose	18120520314	1
Spagyra/Österreich	Sacarose	18120720497	1
Spagyra/Österreich	Sacarose	18121320236	1
Spagyra/Österreich	Sacarose	18121320237	1
Spagyra/Österreich	Sacarose	19010320203	1
Spagyra/Österreich	Sacarose	19010320204	1
Spagyra/Österreich	Sacarose	19010320205	1
Spagyra/Österreich	Sacarose	19010320207	1
Spagyra/Österreich	Sacarose	19010320208	1
Spagyra/Österreich	Sacarose	19010320209	1
Spagyra/Österreich	Sacarose	19011421251	1
Spagyra/Österreich	Sacarose	19020521071	1
Spagyra/Österreich	Sacarose	19020521072	1
Spagyra/Österreich	Sacarose	19043020816	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sacarose	19060620656	1
Spagyra/Österreich	Sacarose	19060720528	1
Spagyra/Österreich	Sacarose	19060720530	1
Spagyra/Österreich	Sacarose	19060720880	1
Spagyra/Österreich	Sacarose	19062120093	1
Spagyra/Österreich	Sacarose	19071020656	1
Spagyra/Österreich	Sacarose	19071020657	1
Spagyra/Österreich	Sacarose	19071020658	1
Spagyra/Österreich	Sacarose	19071020659	1
Spagyra/Österreich	Sacarose	19080520520	1
Spagyra/Österreich	Sacarose	19080720443	1
Spagyra/Österreich	Sacarose	19082621169	1
Spagyra/Österreich	Sacarose	19082621170	1
Spagyra/Österreich	Sacarose	19082621174	1
Spagyra/Österreich	Sacarose	19082621175	1
Spagyra/Österreich	Sacarose	1910320206	1
Spagyra/Österreich	Sacarose	19110420478	1
Spagyra/Österreich	Sacarose	19110720552	1
Spagyra/Österreich	Sacarose	19112220556	1
Spagyra/Österreich	Sacarose	20012420378	1
Spagyra/Österreich	Sacarose	20012420379	1
Spagyra/Österreich	Sacarose	2001290835	1
Spagyra/Österreich	Sacarose	20021120369	1
Spagyra/Österreich	Sacarose	20021120370	1
Spagyra/Österreich	Sacarose	200220020125	1
Spagyra/Österreich	Sacarose	20022620346	1
Spagyra/Österreich	Sacarose	20022620347	1
Spagyra/Österreich	Sacarose	20030220903	1
Spagyra/Österreich	Sacarose	20030220904	1
Spagyra/Österreich	Sacarose	20030520349	1
Spagyra/Österreich	Sacarose	20030520350	1
Spagyra/Österreich	Sacarose	20031120315	1
Spagyra/Österreich	Sacarose	20031120316	1
Spagyra/Österreich	Sacarose	20031820569	1
Spagyra/Österreich	Sacarose	20032321824	1
Spagyra/Österreich	Sacarose	20032420357	1
Spagyra/Österreich	Sacarose	20032420358	1
Spagyra/Österreich	Sacarose	20032420359	1
Spagyra/Österreich	Sacarose	20032520757	1
Spagyra/Österreich	Sacarose	20032520824	1
Spagyra/Österreich	Sacarose	20032520825	1
Spagyra/Österreich	Sacarose	20032520826	1
Spagyra/Österreich	Sacarose	20032520827	1
Spagyra/Österreich	Sacarose	20033120462	1
Spagyra/Österreich	Sacarose	20040120719	1
Spagyra/Österreich	Sacarose	20040820313	1
Spagyra/Österreich	Sacarose	20040820315	1
Spagyra/Österreich	Sacarose	20042020392	2
Spagyra/Österreich	Sacarose	20042020394	1
Spagyra/Österreich	Sacarose	20042020395	1
Spagyra/Österreich	Sacarose	20042020398	1
Spagyra/Österreich	Sacarose	20042020399	1
Spagyra/Österreich	Sacarose	20042020400	1
Spagyra/Österreich	Sacarose	20042020401	1
Spagyra/Österreich	Sacarose	20042020402	1
Spagyra/Österreich	Sacarose	20050520188	1
Spagyra/Österreich	Sacarose	20050520189	1
Spagyra/Österreich	Sacarose	20050520190	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sacarose	20050520191	1
Spagyra/Österreich	Sacarose	20050520193	1
Spagyra/Österreich	Sacarose	20050520194	1
Spagyra/Österreich	Sacarose	20050720449	1
Spagyra/Österreich	Sacarose	20052520367	1
Spagyra/Österreich	Sacarose	20052520368	1
Spagyra/Österreich	Sacarose	20061720426	1
Spagyra/Österreich	Sacarose	20061720427	1
Spagyra/Österreich	Sacarose	20061720428	1
Spagyra/Österreich	Sacarose	20061720480	1
Spagyra/Österreich	Sacarose	20062620145	1
Spagyra/Österreich	Sacarose	20070720637	1
Spagyra/Österreich	Sacarose	20072920245	1
Spagyra/Österreich	Sacarose	20082620273	1
Spagyra/Österreich	Sacarose	20082620274	1
Spagyra/Österreich	Sacarose	20082820224	1
Spagyra/Österreich	Sacarose	20082820225	1
Spagyra/Österreich	Sacarose	20082820226	1
Spagyra/Österreich	Sacarose	20090120367	1
Spagyra/Österreich	Sacarose	20090120368	1
Spagyra/Österreich	Sacarose	20091020538	1
Spagyra/Österreich	Sacarose	20091020539	1
Spagyra/Österreich	Sacarose	20091720367	1
Spagyra/Österreich	Sacarose	20091720374	1
Spagyra/Österreich	Sacarose	20091720375	1
Spagyra/Österreich	Sacarose	20092821146	1
Spagyra/Österreich	Sacarose	20092821147	1
Spagyra/Österreich	Sacarose	20092821149	1
Spagyra/Österreich	Sacarose	20092821152	1
Spagyra/Österreich	Sacarose	20092821153	1
Spagyra/Österreich	Sacarose	20092821154	1
Spagyra/Österreich	Sacarose	20092821155	1
Spagyra/Österreich	Sacarose	20092821156	1
Spagyra/Österreich	Sacarose	20093020124	1
Spagyra/Österreich	Sacarose	20102320364	1
Spagyra/Österreich	Sacarose	20102320365	1
Spagyra/Österreich	Sacarose	20102320366	1
Spagyra/Österreich	Sacarose	20102720460	1
Spagyra/Österreich	Sacarose	20111720437	1
Spagyra/Österreich	Sacarose	20111720439	1
Spagyra/Österreich	Sacarose	20112321275	1
Spagyra/Österreich	Sacarose	20112321277	1
Spagyra/Österreich	Sacarose	20112321278	1
Spagyra/Österreich	Sacarose	20112321279	1
Spagyra/Österreich	Sacarose	20112520599	1
Spagyra/Österreich	Sacarose	20112520600	1
Spagyra/Österreich	Sacarose	20112520601	1
Spagyra/Österreich	Sacarose	20112520602	1
Spagyra/Österreich	Sacarose	20112520603	1
Spagyra/Österreich	Sacarose	20112520604	1
Spagyra/Österreich	Sacarose	20112520605	1
Spagyra/Österreich	Sacarose	20112520606	1
Spagyra/Österreich	Sacarose	20112520607	1
Spagyra/Österreich	Sacarose	20112520608	1
Spagyra/Österreich	Sacarose	20112520609	1
Spagyra/Österreich	Sacarose	20112720457	1
Spagyra/Österreich	Sacarose	20112720459	1
Spagyra/Österreich	Sacarose	20112720460	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sacarose	20112720461	1
Spagyra/Österreich	Sacarose	20122320203	1
Spagyra/Österreich	Sacarose	20122320204	1
Spagyra/Österreich	Sacarose	2042220600	1
Spagyra/Österreich	Sacarose	2042220601	1
Spagyra/Österreich	Sacarose	2042220602	1
Spagyra/Österreich	Sacarose	20881420115	1
Spagyra/Österreich	Sacarose	21011120754	1
Spagyra/Österreich	Sacarose	21011120755	1
Spagyra/Österreich	Sacarose	21011120756	1
Spagyra/Österreich	Sacarose	21012120262	1
Spagyra/Österreich	Sacarose	21022220519	1
Spagyra/Österreich	Sacarose	21022220531	1
Spagyra/Österreich	Sacarose	21022220532	1
Spagyra/Österreich	Sacarose	21022420250	1
Spagyra/Österreich	Sacarose	21030320285	1
Spagyra/Österreich	Sacarose	21030320286	1
Spagyra/Österreich	Sacarose	21030320289	1
Spagyra/Österreich	Sacarose	21031520864	1
Spagyra/Österreich	Sacarose	21031920545	1
Spagyra/Österreich	Sacarose	21033020089	1
Spagyra/Österreich	Sacarose	21042221787	1
Spagyra/Österreich	Sacarose	21042820617	1
Spagyra/Österreich	Sacarose	21050420503	1
Spagyra/Österreich	Sacarose	21051720779	1
Spagyra/Österreich	Sacarose	21051720780	1
Spagyra/Österreich	Sacarose	21051720781	1
Spagyra/Österreich	Sacarose	21051720782	1
Spagyra/Österreich	Sacarose	21051720783	1
Spagyra/Österreich	Sacarose	21051720785	1
Spagyra/Österreich	Sacarose	21051720786	1
Spagyra/Österreich	Sacarose	21061020532	1
Spagyra/Österreich	Sacarose	21061020535	1
Spagyra/Österreich	Sacarose	21072320083	1
Spagyra/Österreich	Sacarose	21072320084	2
Spagyra/Österreich	Sacarose	21090920173	1
Spagyra/Österreich	Sacarose	21090920174	1
Spagyra/Österreich	Sacarose	21090920176	2
Spagyra/Österreich	Sacarose	21090920177	2
Spagyra/Österreich	Sacarose	21101520263	1
Spagyra/Österreich	Sacarose	2307	2
Spagyra/Österreich	Sacarose	2382	1
Spagyra/Österreich	Sacarose	2506	1
Spagyra/Österreich	Sacarose	2516	1
Spagyra/Österreich	Sacarose	2963	1
Spagyra/Österreich	Sacarose	3071	1
Spagyra/Österreich	Sacarose	3082	1
Spagyra/Österreich	Sacarose	3183	1
Spagyra/Österreich	Sacarose	3303	1
Spagyra/Österreich	Sacarose	3802	1
Spagyra/Österreich	Sacarose	3988	1
Spagyra/Österreich	Sacarose	4087	1
Spagyra/Österreich	Sacarose	4153	1
Spagyra/Österreich	Sacarose	4159	1
Spagyra/Österreich	Sacarose	4251	1
Spagyra/Österreich	Sacarose	4255	1
Spagyra/Österreich	Sacarose	4338	1
Spagyra/Österreich	Sacarose	4417	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sacarose	4504	1
Spagyra/Österreich	Sacarose	4941	1
Spagyra/Österreich	Sacarose	4965	1
Spagyra/Österreich	Sacarose	5009	1
Spagyra/Österreich	Sacarose	5030920991	1
Spagyra/Österreich	Sacarose	5030920993	1
Spagyra/Österreich	Sacarose	5030921008	1
Spagyra/Österreich	Sacarose	5030921018	1
Spagyra/Österreich	Sacarose	5031	1
Spagyra/Österreich	Sacarose	5156	1
Spagyra/Österreich	Sacarose	5329	1
Spagyra/Österreich	Sacarose	5520	2
Spagyra/Österreich	Sacarose	5545	1
Spagyra/Österreich	Sacarose	5660	1
Spagyra/Österreich	Sacarose	5699	1
Spagyra/Österreich	Sacarose	5743	1
Spagyra/Österreich	Sacarose	5899	1
Spagyra/Österreich	Sacarose	5998	1
Spagyra/Österreich	Sacarose	6019	1
Spagyra/Österreich	Sacarose	6032	2
Spagyra/Österreich	Sacarose	6047	1
Spagyra/Österreich	Sacarose	6079	1
Spagyra/Österreich	Sacarose	6091	2
Spagyra/Österreich	Sacarose	6106	1
Spagyra/Österreich	Sacarose	6128	1
Spagyra/Österreich	Sacarose	6201	1
Spagyra/Österreich	Sacarose	6243	1
Spagyra/Österreich	Sacarose	6285	1
Spagyra/Österreich	Sacarose	6327	1
Spagyra/Österreich	Sacarose	6340	1
Spagyra/Österreich	Sacarose	6371	1
Spagyra/Österreich	Sacarose	6409	1
Spagyra/Österreich	Sacarose	6415	1
Spagyra/Österreich	Sacarose	6562	1
Spagyra/Österreich	Sacarose	H17-0047	1
Spagyra/Österreich	Sacarose	H18-0021	1
Spagyra/Österreich	Sacarose	H18-0210	1
Spagyra/Österreich	Sacarose	H18-0235	1
Spagyra/Österreich	Sacarose	H18-0252	1
Spagyra/Österreich	Sacarose	H18-0327	1
Spagyra/Österreich	Sacarose	H19-0130	1
Spagyra/Österreich	Sacarose	H19-0270	1
Spagyra	Sacarose	10032921256	1
Spagyra	Sacarose	10073020385	1
Spagyra	Sacarose	12082320717	1
Spagyra	Sacarose	12103020975	1
Spagyra	Sacarose	13012920302	1
Spagyra	Sacarose	13020620240	1
Spagyra	Sacarose	13030621373	1
Spagyra	Sacarose	13040921424	1
Spagyra	Sacarose	13040921427	1
Spagyra	Sacarose	13040921430	1
Spagyra	Sacarose	13040921431	1
Spagyra	Sacarose	13041920152	2
Spagyra	Sacarose	13041920154	1
Spagyra	Sacarose	13050621773	2
Spagyra	Sacarose	13051520939	1
Spagyra	Sacarose	13051520941	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra	Sacarose	13061020524	1
Spagyra	Sacarose	13061020525	1
Spagyra	Sacarose	13061020526	1
Spagyra	Sacarose	13061020528	1
Spagyra	Sacarose	13061020529	1
Spagyra	Sacarose	13061220385	2
Spagyra	Sacarose	13070420936	2
Spagyra	Sacarose	13070420937	2
Spagyra	Sacarose	13070420938	1
Spagyra	Sacarose	13072620834	1
Spagyra	Sacarose	15032620414	1
Spagyra	Sacarose	15082720411	1
Spagyra	Sacarose	16032920732	1
Spagyra	Sacarose	16042522126	1
Spagyra	Sacarose	16050220821	1
Spagyra	Sacarose	16050421023	1
Spagyra	Sacarose	16051820801	1
Spagyra	Sacarose	16053020827	1
Spagyra	Sacarose	16070421669	1
Spagyra	Sacarose	16083120745	1
Spagyra	Sacarose	16102120418	1
Spagyra	Sacarose	16110320884	1
Spagyra	Sacarose	1691	1
Spagyra	Sacarose	17070420968	1
Spagyra	Sacarose	17072120536	1
Spagyra	Sacarose	17072120537	1
Spagyra	Sacarose	17072120538	1
Spagyra	Sacarose	17080920574	1
Spagyra	Sacarose	17082320366	1
Spagyra	Sacarose	17090620617	1
Spagyra	Sacarose	18081720533	1
Spagyra	Sacarose	19043020815	1
Spagyra	Sacarose	1905	1
Spagyra	Sacarose	1911	1
Spagyra	Sacarose	1918	1
Spagyra	Sacarose	2007	2
Spagyra	Sacarose	20102720461	1
Spagyra	Sacarose	20102720462	1
Spagyra	Sacarose	2923	1
Spagyra	Sacarose	3750	1
Spagyra	Sacarose	5030920873	1
Spagyra	Sacarose	5030920881	1
Spagyra	Sacarose	5030920883	1
Spagyra	Sacarose	5030920885	1
Spagyra	Sacarose	5030920893	1
Spagyra	Sacarose	5030920895	1
Spagyra	Sacarose	5030920908	1
Spagyra	Sacarose	5030920922	1
Spagyra	Sacarose	5030920923	1
Spagyra	Sacarose	5030920924	1
Spagyra	Sacarose	5030920989	1
Spagyra	Sacarose	5030920995	1
Spagyra	Sacarose	5030920996	1
Spagyra	Sacarose	5030920997	1
Spagyra	Sacarose	5030920998	1
Spagyra	Sacarose	5030920999	1
Spagyra	Sacarose	5030921002	1
Spagyra	Sacarose	5030921004	1
Spagyra	Sacarose	5030921006	1
Spagyra	Sacarose	5030921010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra	Sacarose	5030921012	1
Spagyra	Sacarose	5030921014	1
Spagyra	Sacarose	5030921015	1
Spagyra	Sacarose	5030921016	1
Spagyra	Sacarose	5030921019	1
Spagyra	Sacarose	5030921020	1
Spagyra	Sacarose	5030921024	1
Spagyra	Sacarose	5030921026	1
Spagyra	Sacarose	5030921028	1
Spagyra	Sacarose	5030921030	1
Spagyra	Sacarose	5030921031	1
Spagyra	Sacarose	5030921032	1
Spagyra	Sacarose	5030921036	1
Spagyra	Sacarose	5030921037	1
Spagyra	Sacarose	5030921038	1
Spagyra	Sacarose	5030921039	1
Spagyra	Sacarose	5030921040	1
Spagyra	Sacarose	5030921041	1
Spagyra	Sacarose	5030921042	1
Spagyra	Sacarose	5030921043	1
Spagyra	Sacarose	5030921053	1
Spagyra	Sacarose	5030921054	1
Spagyra	Sacarose	5030921056	1
Spagyra	Sacarose	5030921060	1
Spagyra	Sacarose	5030921064	1
Spagyra	Sacarose	5030921065	1
Spagyra	Sacarose	5030921067	1
Spagyra	Sacarose	5030921072	1
Spagyra	Sacarose	5030921075	1
Spagyra	Sacarose	5030921078	1
Spagyra	Sacarose	5030921080	1
Spagyra	Sacarose	5030921081	1
Spagyra	Sacarose	5030921082	1
Spagyra	Sacarose	5030921090	1
Spagyra	Sacarose	5030921094	1
Spagyra	Sacarose	5030921096	1
Spagyra	Sacarose	5030921100	1
Spagyra	Sacarose	5030921101	1
Spagyra	Sacarose	5030921122	1
Spagyra	Sacarose	5030921152	1
Spagyra	Sacarose	5030921221	1
Spagyra	Sacarose	7062220875	1
SpagyraÖsterreich	Sacarose	21112620135	1
SpagyraÖsterreich	Sacarose	21112620136	1
SpagyraÖsterreich	Sacarose	21112620137	1
SpagyraÖsterreich	Sacarose	21112620138	1
SpagyraÖsterreich	Sacarose	21112620139	1
SpagyraÖsterreich	Sacarose	21112620140	1
SpagyraÖsterreich	Sacarose	21112620141	1
SpagyraÖsterreich	Sacarose	21120220394	1
SpagyraÖsterreich	Sacarose	21120220395	1
SpagyraÖsterreich	Sacarose	22010420102	1
SpagyraÖsterreich	Sacarose	22010420103	1
SpagyraÖsterreich	Sacarose	22010420104	1
SpagyraÖsterreich	Sacarose	22010420105	1
SpagyraÖsterreich	Sacarose	22010420106	1
SpagyraÖsterreich	Sacarose	22010420107	1
SpagyraÖsterreich	Sacarose	22012520412	1
SpagyraÖsterreich	Sacarose	22020820910	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
SpagyraÖsterreich	Sacarose	22020820911	1
SpagyraÖsterreich	Sacarose	22020821013	1
SpagyraÖsterreich	Sacarose	22020821014	1
SpagyraÖsterreich	Sacarose	22020821015	1
SpagyraÖsterreich	Sacarose	22020821016	1
SpagyraÖsterreich	Sacarose	22021020386	1
SpagyraÖsterreich	Sacarose	22021020387	1
SpagyraÖsterreich	Sacarose	22030000141	2
SpagyraÖsterreich	Sacarose	22031720088	1
SpagyraÖsterreich	Sacarose	22042020195	1
SpagyraÖsterreich	Sacarose	22042020199	1
SpagyraÖsterreich	Sacarose	22042720155	1
SpagyraÖsterreich	Sacarose	22050620618	1
SpagyraÖsterreich	Sacarose	22050620621	2
SpagyraÖsterreich	Sacarose	22050620622	1
SpagyraÖsterreich	Sacarose	22060220035	1
SpagyraÖsterreich	Sacarose	22060220038	1
SpagyraÖsterreich	Sacarose	22060920061	1
SpagyraÖsterreich	Sacarose	22060920062	1
SpagyraÖsterreich	Sacarose	22060920063	1
SpagyraÖsterreich	Sacarose	22060920064	1
SpagyraÖsterreich	Sacarose	22060920065	1
SpagyraÖsterreich	Sacarose	22062020221	1
SpagyraÖsterreich	Sacarose	22070420262	1
SpagyraÖsterreich	Sacarose	22070820291	1
SpagyraÖsterreich	Sacarose	22080220229	1
SpagyraÖsterreich	Sacarose	22080220230	1
SpagyraÖsterreich	Sacarose	22081620115	1
SpagyraÖsterreich	Sacarose	22081620117	1
SpagyraÖsterreich	Sacarose	22083020318	1
SpagyraÖsterreich	Sacarose	22083020323	2
SpagyraÖsterreich	Sacarose	22083020326	1
SpagyraÖsterreich	Sacarose	22090220218	1
SpagyraÖsterreich	Sacarose	22090620388	1
SpagyraÖsterreich	Sacarose	6083	1
SpagyraÖsterreich	Sacarose	6116	1
SpagyraÖsterreich	Sacarose	6553	1
SpagyraÖsterreich	Sacarose	6807	1
SpagyraÖsterreich	Sacarose	680722021720173	1
SpagyraÖsterreich	Sacarose	680722021720174	1
SpagyraÖsterreich	Sacarose	680722021720175	1
SpagyraÖsterreich	Sacarose	680722021720176	1
SpagyraÖsterreich	Sacarose	680722021720177	1
SpagyraÖsterreich	Sacarose	680722021720178	1
SpagyraÖsterreich	Sacarose	7056	1
SpagyraÖsterreich	Sacarose	7075	1
SpagyraÖsterreich	Sacarose	7206	1
SpagyraÖsterreich	Sacarose	7237	1
SpagyraÖsterreich	Sacarose	7263	2
SpagyraÖsterreich	Sacarose	7318	2
SpagyraÖsterreich	Sacarose	7340	1
SpagyraÖsterreich	Sacarose	7377	1
SpagyraÖsterreich	Sacarose	7447	1
SpagyraÖsterreich	Sacarose	7656	1
SpagyraÖsterreich	Sacarose	7660	1
SpagyraÖsterreich	Sacarose	H20-0298	1
St. Erhard Apotheke	Sacarose	1809052072	1
St. Erhard Apotheke	Sacarose	18090520790	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
St. Erhard Apotheke	Sacarose	18090520791	1
St. Erhard Apotheke	Sacarose	18090520792	1
St. Erhard Apotheke	Sacarose	18090520793	1
St. Erhard Apotheke	Sacarose	18090520794	1
St. Erhard Apotheke	Sacarose	18090520795	1
St. Erhard Apotheke	Sacarose	19060720878	1
St. Erhard Apotheke	Sacarose	19061720787	1
St. Erhard Apotheke	Sacarose	19061721186	1
St. Erhard Apotheke	Sacarose	20032321403	1
St. Erhard Apotheke	Sacarose	20032321827	1
St. Erhard Apotheke	Sacarose	20100920507	1
St. Erhard Apotheke	Sacarose	21020520525	1
St. Erhard Apotheke	Sacarose	21020520526	1
St. Erhard Apotheke	Sacarose	21020520527	1
St. Erhard Apotheke	Sacarose	32520757	1
Staufen-Pharma	Sacarose	161112	2
Staufenpharma	Sacarose	3314E-01586	1
südzucker	Sacarose		1
südzucker	Sacarose	L120031600	1
Wepa	Sacarose	LOTAP-SP0005	1
Werner	Sacarose	1901208731	2

- 234 296 spectra from 1515 *Apo-Ident* customers from a total of 48 565 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sacarose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sacarose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	580	0	152 382
Type B	0	340	0	201 744
Type C	0	1771	0	234 296

The substance/substance group *Sacarose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9655 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2353 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.6612 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21484	21484	0,00	51,55
21736	21484	4,20	54,45
22615	22615	0,00	53,90
22643	22643	0,00	57,18
23057	23057	0,00	55,10
23058	23058	0,00	56,32
23297	23297	0,00	54,56
23666	23666	0,00	57,67
23833	23833	0,00	53,22
24217	24217	0,00	58,00
25651	25651	0,00	79,97
26630	26630	0,00	58,45
26723	26723	0,00	64,00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Salicilato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21037-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Salicilato de sódio; Natrii salicylas

Special notes

When selecting the *Salicilato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Salicilato de sódio	4	3	7

Second-stage model

For differentiation of the substance/substance group *Salicilato de sódio* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Salicilato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ditranol	74,88	16,20
⋮	⋮	⋮
Cloreto de dequalínio	>50	50,47
Ácido benzoico	>50	51,09
Ácido acetilsalicílico	>50	104,30
Eosina amarela	>50	156,74
Cloridrato de oxitetraciclina	>50	261,41
Levotiroxina sódica	>50	580,74
Tanino	>50	1207,07

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Salicilato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Salicilato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Salicilato de sódio	12158307	21037	40	1403225
Caelo	Salicilato de sódio	13140513	21689	60	20130531
Caelo	Salicilato de sódio	163053	23052	40	20161118*
Gatt-Koller	Salicilato de sódio	22J02278	26705	40	20221206

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Salicilato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 782 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Salicilato de sódio*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Salicilato de sódio	16305301	22879	40
Caelo	Salicilato de sódio	20002958001	25428	40
Gatt-Koller	Salicilato de sódio	23J02384	27094	40
Gatt-Koller	Salicilato de sódio	22J02278	26705SI†	20
Gatt-Koller	Salicilato de sódio	23J02384	27094SI	20

- 201 924 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 7 batches from the substance/substance group *Salicilato de sódio*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Salicilato de sódio	18061305	1
Caelo	Salicilato de sódio	20002958001	1
Caesar & Loretz GmbH	Salicilato de sódio	20004439001	2
Fagron	Salicilato de sódio	102091210	1
GATT-KOLLER/PHOENIX	Salicilato de sódio	4853/11124512	1
Gehe	Salicilato de sódio	13G31-B03-287961	1
Phoenix	Salicilato de sódio	12158309	1

- 236 059 spectra from 1515 *Apo-Ident* customers from a total of 49 251 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Salicilato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Salicilato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	160	0	201 924
Type C	0	8	0	236 059

The substance/substance group *Salicilato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21037	21037	0,00	197,10
21689	21037	5,69	197,05
23052	23052	0,00	185,91
26705	21037	26,70	181,82

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Serina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	22289-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Serina; Serinum

Special notes

When selecting the *Serina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Serina	8	8	3

Second-stage model

For differentiation of the substance/substance group *Serina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Serina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	81,75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Serina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Serina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Serina	1512012	22289	60	20160112*
Euro OTC	Serina	1606020-01	22668	40	20160714
Euro OTC	Serina	1606020	22678	40	20160714*
Euro OTC	Serina	1711033	23914	40	20171208*
Euro OTC	Serina	1904034	24641	40	20190521*
Euro OTC	Serina	1909027	24956	40	20191015*
Euro OTC	Serina	2011007	25471	40	20201127*
Fagron	Serina	21J20-B02-216460	26156	40	20220114
Fagron	Serina	21J20-B02-216460	26156SI	20	20220114

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Serina*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 602 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 370 spectra of 10 reference samples from the substance/substance group *Serina*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Serina	1611006	22922	40
Euro OTC	Serina	1809016	24296	40
Euro OTC	Serina	2006028	25305	40
Euro OTC	Serina	2107017	25776	50
Euro OTC	Serina	2206022	26275	40
Euro OTC	Serina	2302004	26599	40
Euro OTC	Serina	2308017	27206	40
Fagron	Serina	23J09-B02-235857	27049	40
Euro OTC	Serina	2206022	26275SI	20
Euro OTC	Serina	2302004	26599SI	20

- 201 714 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 2 *Apo-Ident* customers from 4 batches from the substance/substance group *Serina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Serina	1606020-01	3
Euro OTC	Serina	1904034-01	1
Euro OTC	Serina	2006028-01	1
Euro OTC	Serina	2206022-01	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Serina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Serina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	370	0	201 714
Type C	0	6	0	236 061

The substance/substance group *Serina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3784 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22289	22289	0,00	202,35
22668	22678	6,14	208,56
22678	22678	0,00	208,53
23914	23914	0,00	206,60
24641	24641	0,00	209,24
24956	24956	0,00	203,40
25471	25471	0,00	208,75
26156	23914	15,51	208,15

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sorbato de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20020-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sorbato de potássio; Kalii sorbas

Special notes

When selecting the *Sorbato de potássio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sorbato de potássio	9	12	223

Second-stage model

For differentiation of the substance/substance group *Sorbato de potássio* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sorbato de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	124,15	–
⋮	⋮	⋮
Furoato de mometasona	>50	37,68
Sulfato de atropina	>50	101,29
Hidrocortisona	>50	159,33
Citrato monobásico de magnésio, hid…	>50	180,42
Cloridrato de propranolol	>50	281,87
Quinolina amarela	>50	383,81
Escina, hidrossolúvel	>50	425,63
Fenitoína	>50	495,57
Sacarina sódica	>50	584,30
Orotato de cálcio di-hidratado	>50	668,21

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sorbato de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sorbato de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbato de potássio	13224604	21444	60	20130813
Caelo	Sorbato de potássio	163266	23059	40	20170105*
Caelo	Sorbato de potássio	17170008	23585	30	20170711
Caelo	Sorbato de potássio	20001879	25556	40	20200714*
Caelo	Sorbato de potássio	20001880	25630	40	20200714*
Caelo	Sorbato de potássio	23001012	26713	40	20230516*
Caelo	Sorbato de potássio	23001012	26713SI	20	20230516*
Euro OTC	Sorbato de potássio	1508025	21892	60	20150902*
Euro OTC	Sorbato de potássio	1608013	22786	40	20160819*
Euro OTC	Sorbato de potássio	1907023	24764	40	20190802*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 10 reference samples from the substance/substance group *Sorbato de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 552 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 530 spectra of 14 reference samples from the substance/substance group *Sorbato de potássio*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbato de potássio	171700	23638	40
Caelo	Sorbato de potássio	173451	23830	40
Caelo	Sorbato de potássio	181650	24224	40
Caelo	Sorbato de potássio	191072	24539	40
Caelo	Sorbato de potássio	21001391	25700	50
Caelo	Sorbato de potássio	22002065	26244	40
Caelo	Sorbato de potássio	23002441	26944	40
Caelo	Sorbato de potássio	23002442	26961	40
Euro OTC	Sorbato de potássio	1703034	23176	40
Euro OTC	Sorbato de potássio	1710015	23772	40
Euro OTC	Sorbato de potássio	1805029	24126	40
Euro OTC	Sorbato de potássio	1901020	24464	40
Caelo	Sorbato de potássio	22002065	26244SI	20
Caelo	Sorbato de potássio	23002441	26944SI	20

- 201 554 spectra from a total of 4033 batches from further 842 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1921 spectra from 981 *Apo-Ident* customers from 228 batches from the substance/substance group *Sorbato de potássio*.
- Among them are spectra of independent samples from 223 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sorbato de potássio		1
	Sorbato de potássio	10012203	1
	Sorbato de potássio	12211101	2
	Sorbato de potássio	17170017	1
	Sorbato de potássio	19000555010	1
	Sorbato de potássio	20004207005	1
	Sorbato de potássio	20004356001	1
	Sorbato de potássio	22002065002	1
	Sorbato de potássio	22003409002	1
	Sorbato de potássio	22003409004	2
	Sorbato de potássio	22003409007	12
	Sorbato de potássio	22003409010	2
	Sorbato de potássio	22003409013	9
	Sorbato de potássio	22003409014	8
	Sorbato de potássio	23001012004	18
	Sorbato de potássio	23001012010	1
	Sorbato de potássio	922331021	1
/Alliance	Sorbato de potássio	18165010	1
AHD	Sorbato de potássio	13065216	1
AHD	Sorbato de potássio	17170007	1
AHD	Sorbato de potássio	17345116	1
AHD	Sorbato de potássio	216331021	1
AHD	Sorbato de potássio	22003409004	1
AHD	Sorbato de potássio	22003409013	1
AHD	Sorbato de potássio	23001012004	1
Alliance Healthcare	Sorbato de potássio	15382115	1
Alliance Healthcare	Sorbato de potássio	20004207002	1
Allianz	Sorbato de potássio	17170006	1
Anzag 12.01.15	Sorbato de potássio	13224611	1
Anzag	Sorbato de potássio	12211107	1
Anzag	Sorbato de potássio	15382114	2
Anzag	Sorbato de potássio	20004207005	1
Anzag	Sorbato de potássio	23001012004	1
apomix	Sorbato de potássio	13224611	1
apomix	Sorbato de potássio	17345104	1
Bombastus	Sorbato de potássio	1117331022	1
Bombastus	Sorbato de potássio	14380632	1
Caeleo/ Kehr	Sorbato de potássio	20004207002	1
Caelo	Sorbato de potássio		2
Caelo	Sorbato de potássio	1/1/0017	1
Caelo	Sorbato de potássio	10012210	1
Caelo	Sorbato de potássio	10199505	1
Caelo	Sorbato de potássio	111033102	1
Caelo	Sorbato de potássio	1112331024	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbato de potássio	1118331022	1
Caelo	Sorbato de potássio	11192305	3
Caelo	Sorbato de potássio	11214207	1
Caelo	Sorbato de potássio	11261304	3
Caelo	Sorbato de potássio	12059902	1
Caelo	Sorbato de potássio	12059905	2
Caelo	Sorbato de potássio	12059908	2
Caelo	Sorbato de potássio	12059909	4
Caelo	Sorbato de potássio	12059914	2
Caelo	Sorbato de potássio	1205999	1
Caelo	Sorbato de potássio	12211101	10
Caelo	Sorbato de potássio	12211102	4
Caelo	Sorbato de potássio	12211107	16
Caelo	Sorbato de potássio	12211108	2
Caelo	Sorbato de potássio	12211121	4
Caelo	Sorbato de potássio	12211123	1
Caelo	Sorbato de potássio	12345	1
Caelo	Sorbato de potássio	13065204	11
Caelo	Sorbato de potássio	13065205	12
Caelo	Sorbato de potássio	13065211	1
Caelo	Sorbato de potássio	13065216	11
Caelo	Sorbato de potássio	13065217	11
Caelo	Sorbato de potássio	13065222	1
Caelo	Sorbato de potássio	13111409	1
Caelo	Sorbato de potássio	1312024-01	2
Caelo	Sorbato de potássio	13224604	17
Caelo	Sorbato de potássio	13224608	2
Caelo	Sorbato de potássio	13224610	1
Caelo	Sorbato de potássio	13224611	12
Caelo	Sorbato de potássio	13224612	18
Caelo	Sorbato de potássio	13277804	1
Caelo	Sorbato de potássio	1397235	1
Caelo	Sorbato de potássio	14140007	1
Caelo	Sorbato de potássio	14192605	2
Caelo	Sorbato de potássio	143806	1
Caelo	Sorbato de potássio	1438060	2
Caelo	Sorbato de potássio	14380601	18
Caelo	Sorbato de potássio	14380602	2
Caelo	Sorbato de potássio	14380606	9
Caelo	Sorbato de potássio	14380607	10
Caelo	Sorbato de potássio	14380610	13
Caelo	Sorbato de potássio	14380612	2
Caelo	Sorbato de potássio	14380613	1
Caelo	Sorbato de potássio	14380618	1
Caelo	Sorbato de potássio	14380620	6
Caelo	Sorbato de potássio	14380621	11
Caelo	Sorbato de potássio	14380622	12
Caelo	Sorbato de potássio	14380627	10
Caelo	Sorbato de potássio	14380631	1
Caelo	Sorbato de potássio	14380632	23
Caelo	Sorbato de potássio	14380633	16
Caelo	Sorbato de potássio	14380635	8
Caelo	Sorbato de potássio	14382606	1
Caelo	Sorbato de potássio	1438633	1
Caelo	Sorbato de potássio	1508025-01	1
Caelo	Sorbato de potássio	15248203	3
Caelo	Sorbato de potássio	15248204	20
Caelo	Sorbato de potássio	15248205	11
Caelo	Sorbato de potássio	15382103	1
Caelo	Sorbato de potássio	15382105	16

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbato de potássio	15382106	1
Caelo	Sorbato de potássio	15382114	13
Caelo	Sorbato de potássio	15382115	11
Caelo	Sorbato de potássio	1608013-01	1
Caelo	Sorbato de potássio	16156505	4
Caelo	Sorbato de potássio	16326602	4
Caelo	Sorbato de potássio	16326606	20
Caelo	Sorbato de potássio	16326607	17
Caelo	Sorbato de potássio	16326608	21
Caelo	Sorbato de potássio	16326609	20
Caelo	Sorbato de potássio	16326615	1
Caelo	Sorbato de potássio	17170002	4
Caelo	Sorbato de potássio	17170005	1
Caelo	Sorbato de potássio	17170006	13
Caelo	Sorbato de potássio	17170007	26
Caelo	Sorbato de potássio	17170007-20171106Ma1	1
Caelo	Sorbato de potássio	17170008	25
Caelo	Sorbato de potássio	17170012	5
Caelo	Sorbato de potássio	17170013	32
Caelo	Sorbato de potássio	17170014	34
Caelo	Sorbato de potássio	17170015	2
Caelo	Sorbato de potássio	17170016	3
Caelo	Sorbato de potássio	17170016P-190225-3	1
Caelo	Sorbato de potássio	17170017	19
Caelo	Sorbato de potássio	17170018	1
Caelo	Sorbato de potássio	1717008	1
Caelo	Sorbato de potássio	17345103	33
Caelo	Sorbato de potássio	17345104	58
Caelo	Sorbato de potássio	17345105	1
Caelo	Sorbato de potássio	17345113	3
Caelo	Sorbato de potássio	17345116	36
Caelo	Sorbato de potássio	18(19000555006)	1
Caelo	Sorbato de potássio	18165006	32
Caelo	Sorbato de potássio	18165010	56
Caelo	Sorbato de potássio	18165014	25
Caelo	Sorbato de potássio	18165015	31
Caelo	Sorbato de potássio	18165016	2
Caelo	Sorbato de potássio	18165016P-190923-1	1
Caelo	Sorbato de potássio	1816510	1
Caelo	Sorbato de potássio	190000555006	1
Caelo	Sorbato de potássio	190000555010	1
Caelo	Sorbato de potássio	190000555011	2
Caelo	Sorbato de potássio	1900055006	2
Caelo	Sorbato de potássio	1900055011	4
Caelo	Sorbato de potássio	19000555005	4
Caelo	Sorbato de potássio	19000555006	59
Caelo	Sorbato de potássio	190005550066	1
Caelo	Sorbato de potássio	19000555009	1
Caelo	Sorbato de potássio	19000555010	37
Caelo	Sorbato de potássio	19000555011	37
Caelo	Sorbato de potássio	1900055505	2
Caelo	Sorbato de potássio	1900055506	3
Caelo	Sorbato de potássio	1900055510	1
Caelo	Sorbato de potássio	1900555010	1
Caelo	Sorbato de potássio	191072008	1
Caelo	Sorbato de potássio	19107203	3
Caelo	Sorbato de potássio	19107203P-200518-1	1
Caelo	Sorbato de potássio	19107206	1
Caelo	Sorbato de potássio	19107207	2
Caelo	Sorbato de potássio	19107208	41

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbato de potássio	19107280	1
Caelo	Sorbato de potássio	198000555006	1
Caelo	Sorbato de potássio	200004207002	1
Caelo	Sorbato de potássio	200004207005	1
Caelo	Sorbato de potássio	200004356006	1
Caelo	Sorbato de potássio	20004207002	42
Caelo	Sorbato de potássio	20004207005	45
Caelo	Sorbato de potássio	20004356001	36
Caelo	Sorbato de potássio	20004356011	14
Caelo	Sorbato de potássio	2000435611	1
Caelo	Sorbato de potássio	20021112-2	1
Caelo	Sorbato de potássio	2004207002	1
Caelo	Sorbato de potássio	2004207005	3
Caelo	Sorbato de potássio	2004356001	1
Caelo	Sorbato de potássio	200613K1	1
Caelo	Sorbato de potássio	20082001	1
Caelo	Sorbato de potássio	2041402	1
Caelo	Sorbato de potássio	21001391008	2
Caelo	Sorbato de potássio	22002065002	11
Caelo	Sorbato de potássio	22003409001	1
Caelo	Sorbato de potássio	22003409002	2
Caelo	Sorbato de potássio	22003409003	2
Caelo	Sorbato de potássio	22003409004	14
Caelo	Sorbato de potássio	22003409007	12
Caelo	Sorbato de potássio	22003409013	2
Caelo	Sorbato de potássio	22003409014	1
Caelo	Sorbato de potássio	220905(22002065002)	1
Caelo	Sorbato de potássio	23001012004	1
Caelo	Sorbato de potássio	27101705	1
Caelo	Sorbato de potássio	317331021	2
Caelo	Sorbato de potássio	3354	1
Caelo	Sorbato de potássio	3512M-01748	1
Caelo	Sorbato de potássio	7111805	1
Caelo	Sorbato de potássio	8165015	1
Caelo	Sorbato de potássio	90318101	1
Caelo	Sorbato de potássio	9061806	1
Caelo	Sorbato de potássio	912331023	1
Caelo	Sorbato de potássio	91623299	2
Caelo	Sorbato de potássio	9305601	2
Caelo	Sorbato de potássio	AKD10	1
Caelo	Sorbato de potássio	K-010213-1	1
Caelo	Sorbato de potássio	RT287	1
Caelo	Sorbato de potássio	RT5324	1
Caesar & Lorenz GmbH	Sorbato de potássio	19000555006	1
Caesar & Lorenz/Noweda	Sorbato de potássio	20004356001	1
Caesar & Loretz GmbH…	Sorbato de potássio	171700006	1
Caesar & Loretz GmbH…	Sorbato de potássio	19107208	2
Caesar & Loretz GmbH…	Sorbato de potássio	15382114	1
Caesar & Loretz GmbH…	Sorbato de potássio	17345103	1
Caesar & Loretz GmbH…	Sorbato de potássio	18165015	1
Caesar & Loretz GmbH…	Sorbato de potássio	20004207005	1
Caesar & Loretz GmbH…	Sorbato de potássio	20004356011	1
Caesar & Loretz GmbH…	Sorbato de potássio	20004207005	1
Caesar & Loretz GmbH…	Sorbato de potássio	13065217	2
Caesar & Loretz GmbH…	Sorbato de potássio	19000555010	1
Caesar & Loretz GmbH…	Sorbato de potássio	20004356011	1
Caesar & Loretz GmbH…	Sorbato de potássio	22003409004	1
Caesar & Loretz GmbH…	Sorbato de potássio	19000555010	1
Caesar & Loretz GmbH…	Sorbato de potássio	17170017	1
Caesar & Loretz GmbH/AHD	Sorbato de potássio	19107203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Sorbato de potássio	19000555010	1
Caesar & Loretz GmbH...	Sorbato de potássio	18165015	1
Caesar & Loretz GmbH...	Sorbato de potássio	20004207002	1
Caesar & Loretz GmbH...	Sorbato de potássio	1900055510	1
Caesar & Loretz GmbH/Gehe	Sorbato de potássio	18165014	1
Caesar & Loretz GmbH/Gehe	Sorbato de potássio	190000555006	1
Caesar & Loretz GmbH/Gehe	Sorbato de potássio	19000555006	1
Caesar & Loretz GmbH/Gehe	Sorbato de potássio	20004207002	1
Caesar & Loretz GmbH/Gehe	Sorbato de potássio	20004207005	2
Caesar & Loretz GmbH/Gehe	Sorbato de potássio	22003409014	1
Caesar & Loretz GmbH...	Sorbato de potássio	20004207002	1
Caesar & Loretz GmbH/K	Sorbato de potássio	19107208	1
Caesar & Loretz GmbH/Kehr	Sorbato de potássio	19000555010	1
Caesar & Loretz GmbH...	Sorbato de potássio	19107208	1
Caesar & Loretz GmbH/Now	Sorbato de potássio	20004207005	1
Caesar & Loretz GmbH...	Sorbato de potássio	19000555006	2
Caesar & Loretz GmbH...	Sorbato de potássio	20004207002	1
Caesar & Loretz GmbH...	Sorbato de potássio	20004356011	1
Caesar & Loretz GmbH...	Sorbato de potássio	19000555011	1
Caesar & Loretz GmbH...	Sorbato de potássio	20004207002	1
Caesar & Loretz GmbH...	Sorbato de potássio	20004356001	1
Caesar & Loretz GmbH...	Sorbato de potássio	22003409003	1
Caesar & Loretz GmbH...	Sorbato de potássio	17345104	1
Caesar & Loretz GmbH...	Sorbato de potássio	18165014	1
Caesar & Loretz GmbH...	Sorbato de potássio	19000555008	1
Caesar & Loretz GmbH...	Sorbato de potássio	19107208	2
Caesar & Loretz GmbH...	Sorbato de potássio	20004207002	1
Caesar & Loretz GmbH...	Sorbato de potássio	22003409002	1
Caesar & Loretz GmbH	Sorbato de potássio	11261303	1
Caesar & Loretz GmbH	Sorbato de potássio	14380627	1
Caesar & Loretz GmbH	Sorbato de potássio	17170006	1
Caesar & Loretz GmbH	Sorbato de potássio	17345103	1
Caesar & Loretz GmbH'	Sorbato de potássio	17345109	2
Caesar & Loretz GmbH	Sorbato de potássio	18165002	1
Caesar & Loretz GmbH	Sorbato de potássio	18165004	1
Caesar & Loretz GmbH	Sorbato de potássio	18165006	1
Caesar & Loretz GmbH	Sorbato de potássio	18165010	12
Caesar & Loretz GmbH	Sorbato de potássio	18165014	4
Caesar & Loretz GmbH	Sorbato de potássio	18165015	6
Caesar & Loretz GmbH	Sorbato de potássio	19000555005	3
Caesar & Loretz GmbH	Sorbato de potássio	19000555006	17
Caesar & Loretz GmbH	Sorbato de potássio	19000555008	3
Caesar & Loretz GmbH	Sorbato de potássio	19000555009	3
Caesar & Loretz GmbH	Sorbato de potássio	19000555010	10
Caesar & Loretz GmbH	Sorbato de potássio	19000555011	6
Caesar & Loretz GmbH	Sorbato de potássio	19107203	1
Caesar & Loretz GmbH	Sorbato de potássio	19107208	15
Caesar & Loretz GmbH	Sorbato de potássio	20001879002	2
Caesar & Loretz GmbH	Sorbato de potássio	20004207002	24
Caesar & Loretz GmbH	Sorbato de potássio	20004207005	11
Caesar & Loretz GmbH	Sorbato de potássio	20004207006	2
Caesar & Loretz GmbH	Sorbato de potássio	20004356001	15
Caesar & Loretz GmbH	Sorbato de potássio	20004356003	2
Caesar & Loretz GmbH	Sorbato de potássio	20004356011	4
Caesar & Loretz GmbH	Sorbato de potássio	20004498001	1
Caesar & Loretz GmbH	Sorbato de potássio	22002065002	5
Caesar & Loretz GmbH	Sorbato de potássio	22002065003	1
Caesar & Loretz GmbH	Sorbato de potássio	22003409002	5
Caesar & Loretz GmbH	Sorbato de potássio	22003409004	3
Caesar & Loretz GmbH	Sorbato de potássio	22003409007	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sorbato de potássio	22003409013	1
Caesar & Loretz GmbH…	Sorbato de potássio	19000555011	1
Caesar & Loretz GmbH…	Sorbato de potássio	22002065002	1
Caesar & Loretz/Geil…	Sorbato de potássio	19000555006	1
Caesar & Loretz/Noweda	Sorbato de potássio	14380621	1
Caesar & Loretz/Noweda	Sorbato de potássio	19000555010	1
Caesar & Loretz/Sanacorp	Sorbato de potássio	17345104	1
Caesar & Loretz	Sorbato de potássio	14380606	2
Caesar & Loretz	Sorbato de potássio	14380633	1
Caesar & Loretz	Sorbato de potássio	17345103	1
Caesar & Loretz	Sorbato de potássio	19000555010	1
Caesar / Gehe	Sorbato de potássio	14380622	1
Caesar und Loretz	Sorbato de potássio	18165010	1
Caesar&Loretz GmbH/S…	Sorbato de potássio	14380607	1
Caesar&Loretz GmbH	Sorbato de potássio	14380622	1
Caesar&Loretz GmbH	Sorbato de potássio	17170014	1
Caesar/Gehe	Sorbato de potássio	19107208	1
Caesar/Lorenz	Sorbato de potássio	13065204	1
Caleo/Krieger	Sorbato de potássio	20004356001	1
canea, gehe	Sorbato de potássio	13065215	1
Cealo/ Noweda	Sorbato de potássio	17345103	1
cealo	Sorbato de potássio	16326607	1
Cealo	Sorbato de potássio	16326609	1
Cealo	Sorbato de potássio	1710013	1
Euro OTC	Sorbato de potássio	1111038-01	1
Euro OTC	Sorbato de potássio	111103802	1
Euro OTC	Sorbato de potássio	1111038-02	2
Euro OTC	Sorbato de potássio	1312024-01	3
Euro OTC	Sorbato de potássio	13224612	1
Euro OTC	Sorbato de potássio	14380622	1
Euro OTC	Sorbato de potássio	14380632	2
Euro OTC	Sorbato de potássio	1508025-01	7
Euro OTC	Sorbato de potássio	15382115	1
Euro OTC	Sorbato de potássio	1608013-01	8
Euro OTC	Sorbato de potássio	1710012-01	1
Euro OTC	Sorbato de potássio	1710015-01	1
Euro OTC	Sorbato de potássio	17170008	1
Euro OTC	Sorbato de potássio	17170013	1
Euro OTC	Sorbato de potássio	1805029-01	1
Euro OTC	Sorbato de potássio	180529-01	1
Euro OTC	Sorbato de potássio	1901020-01	5
Euro OTC	Sorbato de potássio	1907023-01	1
Euro OTC	Sorbato de potássio	1907023-02	1
Euro OTC	Sorbato de potássio	1991020-01	1
Euro OTC	Sorbato de potássio	216331021	1
Euro OTC	Sorbato de potássio	PS20180905	1
Fagron	Sorbato de potássio	1114331022	1
Fagron	Sorbato de potássio	13065217	1
Fagron	Sorbato de potássio	14380622	1
Fagron	Sorbato de potássio	16326609	1
Fagron	Sorbato de potássio	17170008	1
Fagron	Sorbato de potássio	17170013	2
Fagron	Sorbato de potássio	17170014	1
Fagron	Sorbato de potássio	2717M-01748	1
Fagron	Sorbato de potássio	3115M-01748	1
Fagron	Sorbato de potássio	3518A-01748	1
Fagron	Sorbato de potássio	3912A-01748	1
Fagron	Sorbato de potássio	4314U-01748	1
Fresenius	Sorbato de potássio	220214221	1
Gehe / Spinnrad	Sorbato de potássio	216331021	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Sorbato de potássio	11261304	1
Gehe	Sorbato de potássio	123331021	1
Gehe	Sorbato de potássio	13065205	1
Gehe	Sorbato de potássio	13065216	1
Gehe	Sorbato de potássio	14380601	1
Gehe	Sorbato de potássio	14380607	1
Gehe	Sorbato de potássio	14380632	1
Gehe	Sorbato de potássio	16326606	1
Gehe	Sorbato de potássio	17170007	2
GEHE	Sorbato de potássio	17170008	1
Gehe	Sorbato de potássio	17170013	1
gehe	Sorbato de potássio	17170014	1
Gehe	Sorbato de potássio	17345116	1
Gehe	Sorbato de potássio	18165010	1
Gehe	Sorbato de potássio	18165014	1
Gehe	Sorbato de potássio	19000555006	1
Gehe	Sorbato de potássio	200004207005	1
Gehe	Sorbato de potássio	20004207005	1
Gehe	Sorbato de potássio	22003409004	1
Gehe	Sorbato de potássio	22003409007	1
GEHE	Sorbato de potássio	22003409007	1
Gehe	Sorbato de potássio	23001012004	1
Geibo	Sorbato de potássio	17170013	1
Ichthyol/Noweda	Sorbato de potássio	13224604	1
Ichthyol-Gesellschaf…	Sorbato de potássio	18165014	1
Jenne	Sorbato de potássio	17170007	1
Jenne	Sorbato de potássio	22003409013	1
jenne	Sorbato de potássio	922331021	1
Kehr/Spinnrad	Sorbato de potássio	317331021	1
Kehr	Sorbato de potássio	16326607	1
Kehr	Sorbato de potássio	18165006	1
Kehr	Sorbato de potássio	22003409013	1
Kehr	Sorbato de potássio	23001012004	1
Noweda / Spinnrad	Sorbato de potássio	216331021	1
Noweda/ Spinnrad	Sorbato de potássio	218331021	1
Noweda/Caesar & Lore…	Sorbato de potássio	22003409004	1
Noweda/Spinnrad GmbH	Sorbato de potássio	322331021	1
Noweda/Spinnrad	Sorbato de potássio	19170208	1
Noweda	Sorbato de potássio	12211101	1
Noweda	Sorbato de potássio	13065222	1
Noweda	Sorbato de potássio	15382115	1
Noweda	Sorbato de potássio	16326606	1
Noweda	Sorbato de potássio	17170014	1
Noweda	Sorbato de potássio	17170017	1
Noweda	Sorbato de potássio	17345103	1
Noweda	Sorbato de potássio	17345116	1
Noweda	Sorbato de potássio	18165010	4
Noweda	Sorbato de potássio	20004207005	3
Noweda	Sorbato de potássio	22003409014	1
Noweda	Sorbato de potássio	23001012004	3
p&m cosmetics/gehe	Sorbato de potássio	17170014	1
Phoenix	Sorbato de potássio	1117331022	1
Phoenix	Sorbato de potássio	1397235	1
Phoenix	Sorbato de potássio	14380627	1
Phoenix	Sorbato de potássio	17170012	1
Phoenix	Sorbato de potássio	17170017	1
Phoenix	Sorbato de potássio	17345104	1
Phoenix	Sorbato de potássio	20004207002	1
Phoenix	Sorbato de potássio	20004207005	1
Phoenix	Sorbato de potássio	216331021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Sorbato de potássio	22002065002	1
Phönix/Spinnrad	Sorbato de potássio	1117331022	2
phönix	Sorbato de potássio	14380632	1
Phönix	Sorbato de potássio	16326607	1
phönix	Sorbato de potássio	16326608	1
Phönix	Sorbato de potássio	17345116	1
PHÖNIX	Sorbato de potássio	19000555006	1
Phönix	Sorbato de potássio	19000555011	1
Phönix	Sorbato de potássio	20004207002	1
Phönix	Sorbato de potássio	201103010	1
Phönix	Sorbato de potássio	22003409014	1
s.Prüfprotokoll	Sorbato de potássio		1
sana	Sorbato de potássio	13224612	1
Sanacorp 29.10.18 EK 4,30	Sorbato de potássio	17345104	1
Sanacorp	Sorbato de potássio	1118331022	1
Sanacorp	Sorbato de potássio	12211101	1
Sanacorp	Sorbato de potássio	13065217	1
Sanacorp	Sorbato de potássio	13224611	1
Sanacorp	Sorbato de potássio	14380610	1
Sanacorp	Sorbato de potássio	17170007	1
Sanacorp	Sorbato de potássio	17170014	1
Sanacorp	Sorbato de potássio	19107208	3
Sanacorp	Sorbato de potássio	20004207005	1
Sanacorp	Sorbato de potássio	22003409014	1
Sanacorp	Sorbato de potássio	23001012004	3
sanacorp	Sorbato de potássio	2300102004	1
Sanacorp	Sorbato de potássio	322331021	1
siehe WE-Prüfprotokoll	Sorbato de potássio	61/11	1
Sonnenberg-Apotheke	Sorbato de potássio	13224604	1
Spinnrad - Noweda	Sorbato de potássio	315331021	1
Spinnrad / Gehe	Sorbato de potássio	317331021	2
Spinnrad / Gehe	Sorbato de potássio	616331022	1
Spinnrad GmbH / Nowe…	Sorbato de potássio	1117331022	1
Spinnrad GmbH Bad Se…	Sorbato de potássio	1019331022	1
Spinnrad GmbH Bad Se…	Sorbato de potássio	1118331022	1
Spinnrad GmbH	Sorbato de potássio	111033102	1
Spinnrad GmbH	Sorbato de potássio	1114331022	1
Spinnrad GmbH	Sorbato de potássio	214331021	1
spinnrad GmbH	Sorbato de potássio	616331022	1
Spinnrad GmbH	Sorbato de potássio	912331023	2
Spinnrad Noweda	Sorbato de potássio	520331021	1
Spinnrad Noweda	Sorbato de potássio	7203311027	1
Spinnrad/ Gehe 18.01.19	Sorbato de potássio	317331021	1
Spinnrad/ Noweda/ 26…	Sorbato de potássio	319331021	1
Spinnrad/ Phönix	Sorbato de potássio	322331021	1
spinnrad/gehe	Sorbato de potássio	216331021	1
Spinnrad/Gehe	Sorbato de potássio	315331021	1
spinnrad/Noweda	Sorbato de potássio	1019331022	1
Spinnrad/Noweda	Sorbato de potássio	1117331022	2
Spinnrad/Noweda	Sorbato de potássio	1118331022	2
Spinnrad/Noweda	Sorbato de potássio	218331021	1
Spinnrad/Noweda	Sorbato de potássio	520331021	1
Spinnrad/Noweda	Sorbato de potássio	720331022	1
Spinnrad/Noweda	Sorbato de potássio	922331021	1
Spinnrad/Phoenix	Sorbato de potássio	1019331022	1
Spinnrad/Phoenix	Sorbato de potássio	317331021	1
Spinnrad/Phönix	Sorbato de potássio	1019331022	1
Spinnrad/Phönix	Sorbato de potássio	1118331022	1
Spinnrad/Phönix	Sorbato de potássio	218331021	1
Spinnrad/Phönix	Sorbato de potássio	319331021	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spinnrad/Sannacorp	Sorbato de potássio	616331022	1
Spinnrad	Sorbato de potássio	111033102	1
spinnrad	Sorbato de potássio	1114331022	1
Spinnrad	Sorbato de potássio	1114331022	3
spinnrad	Sorbato de potássio	1117331022	1
Spinnrad	Sorbato de potássio	1117331022	2
spinnrad	Sorbato de potássio	1118331022	1
Spinnrad	Sorbato de potássio	1118331022	1
Spinnrad	Sorbato de potássio	214331021	1
spinnrad	Sorbato de potássio	216331021	1
Spinnrad	Sorbato de potássio	216331021	2
spinnrad	Sorbato de potássio	2233102	1
Spinnrad	Sorbato de potássio	312331021	2
Spinnrad	Sorbato de potássio	315331021	2
spinnrad	Sorbato de potássio	317331021	1
Spinnrad	Sorbato de potássio	317331021	3
spinnrad	Sorbato de potássio	520331021	1
Spinnrad	Sorbato de potássio	520331021	3
spinnrad	Sorbato de potássio	616331022	1
Spinnrad	Sorbato de potássio	616331022	2
spinnrad	Sorbato de potássio	720331022	2
Spinnrad	Sorbato de potássio	720331022	1
Spinnrad	Sorbato de potássio	815331022	2
Spinnrad	Sorbato de potássio	912331023	4
Spinrad/Phönix	Sorbato de potássio	218331021	1
WE: über Eyach 5g/2,...	Sorbato de potássio	14380601	1
wie gehbat	Sorbato de potássio	wiegehabt	1

- 234 146 spectra from 1515 *Apo-Ident* customers from a total of 49 034 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sorbato de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sorbato de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	530	0	201 554
Type C	0	1919	2	234 146

The substance/substance group *Sorbato de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8679 %)
Type C	100.0000 % (> 99.9007 %)	99.8959 % (> 99.7397 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21444	21892	15,19	200,11
21892	21892	0,00	198,68
22786	22786	0,00	196,67
23059	23059	0,00	207,15
23585	25630	19,20	205,30
24764	24764	0,00	197,95
25556	25556	0,00	204,01
25630	25630	0,00	204,51
26713	26713	0,00	203,18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sorbitol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20075-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sorbitol

Special notes

When selecting the *Sorbitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sorbitol	9	14	151

Second-stage model

For differentiation of the substance/substance group *Sorbitol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sorbitol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Xilitol	68,08	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sorbitol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sorbitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbitol	13278217	21485	40	20130920
Caelo	Sorbitol	16038501	22847	40	20160315
Caelo	Sorbitol	163531	23028	40	20170119*
Caelo	Sorbitol	16353107	23442	40	20170119
Caelo	Sorbitol	20001873	25226	40	20200722*
Euro OTC	Sorbitol	1506052	21834	60	20150713*
Euro OTC	Sorbitol	1512016	22293	60	20160113*
Euro OTC	Sorbitol	1604007	22539	40	20160428*
Euro OTC	Sorbitol	1610018	22849	40	20161121*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Sorbitol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 680 spectra of 20 reference samples from the substance/substance group *Sorbitol*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbitol	181636	24220	40
Caelo	Sorbitol	190173	24562	40
Caelo	Sorbitol	192579	24898	40
Caelo	Sorbitol	22003595	26503	40
Caelo	Sorbitol	23000792	26707	40
Caelo	Sorbitol	24000391	27252	40
Euro OTC	Sorbitol	1810010	24306	40
Euro OTC	Sorbitol	2008016	25333	40
Euro OTC	Sorbitol	2108021	25878	50
Euro OTC	Sorbitol	2207023	26271	40
Euro OTC	Sorbitol	2407005	27396	40
Euro OTC	Sorbitol	2411016	27463	40
Fagron	Sorbitol	22B07-B02-218419	26153	40
Fagron	Sorbitol	22J22-B02	26446	40
Caelo	Sorbitol	22003595	26503SI	20
Euro OTC	Sorbitol	2108021	25878SI	10
Euro OTC	Sorbitol	2207023	26271SI	20
Euro OTC	Sorbitol	2407005	27396SI	20
Euro OTC	Sorbitol	2411016	27463SI	20
Fagron	Sorbitol	22B07-B02-218419	26153SI	20

- 201 404 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 459 spectra from 187 *Apo-Ident* customers from 156 batches from the substance/substance group *Sorbitol*.
- Among them are spectra of independent samples from 150 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sorbitol	21003580009	1
	Sorbitol	2108021-01	1
	Sorbitol	22003595002	1
	Sorbitol	22003595005	4
	Sorbitol	22003595007	1
	Sorbitol	22003595008	2
	Sorbitol	22003595009	1
	Sorbitol	23000792004	1
Bombastus	Sorbitol	13278206	2
Caela/ L2	Sorbitol	16038501	1
Caelo	Sorbitol		1
Caelo	Sorbitol	10383323	1
Caelo	Sorbitol	1083330	1
Caelo	Sorbitol	113793	1
Caelo	Sorbitol	11379320	1
Caelo	Sorbitol	11379321	1
Caelo	Sorbitol	11379322	1
Caelo	Sorbitol	11379332	2
Caelo	Sorbitol	11379333	1
Caelo	Sorbitol	11379336	2
Caelo	Sorbitol	11379337	2
Caelo	Sorbitol	12249108	2
Caelo	Sorbitol	12249109	2
Caelo	Sorbitol	12249110	4
Caelo	Sorbitol	12249124	2
Caelo	Sorbitol	12249126	2
Caelo	Sorbitol	12249139	1
Caelo	Sorbitol	12249140	1
Caelo	Sorbitol	12345	1
Caelo	Sorbitol	12L07-N12	1
Caelo	Sorbitol	13278204	1
Caelo	Sorbitol	13278206	1
Caelo	Sorbitol	13278216	2
Caelo	Sorbitol	13278218	1
Caelo	Sorbitol	13278239	1
Caelo	Sorbitol	13278241	1
Caelo	Sorbitol	13278246	2
Caelo	Sorbitol	13278247	1
Caelo	Sorbitol	13278249	1
Caelo	Sorbitol	13278250	1
Caelo	Sorbitol	133335307	1
Caelo	Sorbitol	13335304	1
Caelo	Sorbitol	13335307	3
Caelo	Sorbitol	14250806	1
Caelo	Sorbitol	14250807	1
Caelo	Sorbitol	14250808	1
Caelo	Sorbitol	15012708	1
Caelo	Sorbitol	15118901	3
Caelo	Sorbitol	15118902	2
Caelo	Sorbitol	15118912	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbitol	1512016-01	2
Caelo	Sorbitol	15208302	4
Caelo	Sorbitol	15208303	1
Caelo	Sorbitol	15208305	4
Caelo	Sorbitol	15208306	4
Caelo	Sorbitol	15208309	3
Caelo	Sorbitol	15208310	5
Caelo	Sorbitol	15208311	3
Caelo	Sorbitol	16038501	5
Caelo	Sorbitol	16038502	3
Caelo	Sorbitol	16038503	1
Caelo	Sorbitol	16038514	9
Caelo	Sorbitol	16038515	9
Caelo	Sorbitol	1604007-01	1
Caelo	Sorbitol	1610018-01	1
Caelo	Sorbitol	16101303	1
Caelo	Sorbitol	16231208	1
Caelo	Sorbitol	162353107	1
Caelo	Sorbitol	16353102	3
Caelo	Sorbitol	16353107	2
Caelo	Sorbitol	16353108	6
Caelo	Sorbitol	17011305	1
Caelo	Sorbitol	17140902	9
Caelo	Sorbitol	17140903	14
Caelo	Sorbitol	17140904	2
Caelo	Sorbitol	1714090903	1
Caelo	Sorbitol	17366301	15
Caelo	Sorbitol	17366304	9
Caelo	Sorbitol	17366305	2
Caelo	Sorbitol	18163605	2
Caelo	Sorbitol	18163606	9
Caelo	Sorbitol	18163607	9
Caelo	Sorbitol	181636606	1
Caelo	Sorbitol	18281603	2
Caelo	Sorbitol	18281605	5
Caelo	Sorbitol	18281605P-190624-2	1
Caelo	Sorbitol	18281610	2
Caelo	Sorbitol	19017304	5
Caelo	Sorbitol	19017305	1
Caelo	Sorbitol	19017307	7
Caelo	Sorbitol	19017308	1
Caelo	Sorbitol	19017312	5
Caelo	Sorbitol	192579001	4
Caelo	Sorbitol	192579002	1
Caelo	Sorbitol	192579006	2
Caelo	Sorbitol	192579007	4
Caelo	Sorbitol	200003822010	1
Caelo	Sorbitol	2000322010	1
Caelo	Sorbitol	20003822001	3
Caelo	Sorbitol	20003822005	6
Caelo	Sorbitol	20003822006	1
Caelo	Sorbitol	20003822008	1
Caelo	Sorbitol	20003822010	2
Caelo	Sorbitol	20003822011	1
Caelo	Sorbitol	20021501	1
Caelo	Sorbitol	2003822012	1
Caelo	Sorbitol	21003580001	2
Caelo	Sorbitol	21003580007	1
Caelo	Sorbitol	21003580008	1
Caelo	Sorbitol	225282222169	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbitol	23071201	1
Caelo	Sorbitol	23081401	1
Caelo	Sorbitol	26071402	1
Caelo	Sorbitol	4091401	1
Caelo	Sorbitol	5021307	1
Caelo	Sorbitol	8081402	1
Caesar & Loretz GmbH...	Sorbitol	19017307	1
Caesar & Loretz GmbH...	Sorbitol	192579007	1
Caesar & Loretz GmbH...	Sorbitol	18163607	1
Caesar & Loretz GmbH...	Sorbitol	18281603	1
Caesar & Loretz GmbH...	Sorbitol	19017305	1
Caesar & Loretz GmbH...	Sorbitol	19017307	4
Caesar & Loretz GmbH/Gehe	Sorbitol	19017307	2
Caesar & Loretz GmbH/Gehe	Sorbitol	19017312	1
Caesar & Loretz GmbH/Gehe	Sorbitol	192579007	1
Caesar & Loretz GmbH/Gehe	Sorbitol	20003822008	2
Caesar & Loretz GmbH...	Sorbitol	19017302	2
Caesar & Loretz GmbH...	Sorbitol	19017308	5
Caesar & Loretz GmbH...	Sorbitol	192579002	1
Caesar & Loretz GmbH	Sorbitol	18163606	2
Caesar & Loretz GmbH	Sorbitol	18163607	1
Caesar & Loretz GmbH	Sorbitol	18281602	3
Caesar & Loretz GmbH	Sorbitol	18281605	4
Caesar & Loretz GmbH	Sorbitol	19017302	1
Caesar & Loretz GmbH	Sorbitol	19017304	1
Caesar & Loretz GmbH	Sorbitol	19017307	2
Caesar & Loretz GmbH	Sorbitol	19017312	4
Caesar & Loretz GmbH	Sorbitol	192579002	2
Caesar & Loretz GmbH	Sorbitol	192579004	2
Caesar & Loretz GmbH	Sorbitol	192579006	3
Caesar & Loretz GmbH	Sorbitol	20003822001	2
Caesar & Loretz GmbH	Sorbitol	20003822010	1
Caesar & Loretz GmbH	Sorbitol	21003580008	4
Caesar & Loretz GmbH	Sorbitol	21003580009	1
Caesar u. Loretz GmbH	Sorbitol	20003822006	1
Caesar u. Loretz GmbH	Sorbitol	20003822016	2
EuRho/Anzag	Sorbitol	3518E-02298	1
EuRho/Anzag	Sorbitol	4712I-02298	1
eurho	Sorbitol	1301019-01	1
EuRho	Sorbitol	161001802	1
Euro OTC	Sorbitol		1
Euro OTC	Sorbitol	1301019-01	3
Euro OTC	Sorbitol	1311034-01	2
Euro OTC	Sorbitol	1404007-01	2
Euro OTC	Sorbitol	1406014-01	1
Euro OTC	Sorbitol	1501048-01	4
Euro OTC	Sorbitol	1506052-01	4
Euro OTC	Sorbitol	150652-01	1
Euro OTC	Sorbitol	1512016-01	4
Euro OTC	Sorbitol	1604007-01	4
Euro OTC	Sorbitol	1610018-01	16
Euro OTC	Sorbitol	1610018-02	3
Euro OTC	Sorbitol	1610018-03	8
Euro OTC	Sorbitol	1810010-01	2
Euro OTC	Sorbitol	1810010-02	2
Euro OTC	Sorbitol	2008016-01	2
Euro OTC	Sorbitol	2008016-02	1
Euro OTC	Sorbitol	200816-01	1
Euro OTC	Sorbitol	2108021-01	1
Euro OTC	Sorbitol	3217M-02298	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sorbitol	3617I-02298	1
Euro OTC	Sorbitol	700476	1
Fagron	Sorbitol		1
Fagron	Sorbitol	11I09-N11	1
Fagron	Sorbitol	12E30-N24	3
Fagron	Sorbitol	12J15-N01	1
Fagron	Sorbitol	12L17-N12	3
Fagron	Sorbitol	13278249	1
Fagron	Sorbitol	13D08-N27	1
Fagron	Sorbitol	13E07-B40	2
Fagron	Sorbitol	13G04-N04	1
Fagron	Sorbitol	14E21-B02	1
Fagron	Sorbitol	M721140	1
Fagron	Sorbitol	M721140/12L17-N12	1
Gatt-Koller / Phoenix	Sorbitol	1718/0513	1
Gatt-Koller / Phoenix	Sorbitol	1718/05134013	1
Gehe 01.09.2014	Sorbitol	13278217	1
GEHE 28.11.2014	Sorbitol	13278245	1
GEHE	Sorbitol	16353108	1
Gehe	Sorbitol	18163606	1
GEHE	Sorbitol	19017305	1
Gehe	Sorbitol	21003580009	1
Gehe	Sorbitol	22003595005	1
Gehe	Sorbitol	22003595007	1
Gehe	Sorbitol	22003595008	1
Hänseler	Sorbitol		1
Herba ACM	Sorbitol	22J01085	1
Jenne	Sorbitol	22003595008	1
L10	Sorbitol	16353108	1
L12	Sorbitol	17140904	3
Merck	Sorbitol	13D08-N27	1
Noweda/ Ichthyol	Sorbitol	1512016-01	1
Noweda	Sorbitol	17140903	1
Noweda	Sorbitol	22003595008	1
Phoenix 12.08.2013	Sorbitol	12249108	1
PHÖNIX	Sorbitol	18281603	1
phönix	Sorbitol	21003580002	1
Sana	Sorbitol	18281603	1
Sanacorp	Sorbitol	1610018-01	1
Sanacorp	Sorbitol	16353107	1
siehe Protokoll	Sorbitol	15208310	1
Spangro 17.05.19	Sorbitol	17140902	1

- 235 608 spectra from 1515 *Apo-Ident* customers from a total of 49 107 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sorbitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sorbitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	680	0	201 404
Type C	0	459	0	235 608

The substance/substance group *Sorbitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1176 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6928 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21485	21834	6,05	90,97
21834	21834	0,00	95,64
22293	22293	0,00	89,03
22539	22539	0,00	88,60
22847	21834	3,13	91,92
22849	22849	0,00	88,85
23028	23028	0,00	96,66
23442	21834	5,76	96,72
25226	25226	0,00	110,16

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfacetamida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20695-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfacetamida; Sulfacetamidum

Special notes

When selecting the *Sulfacetamida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfacetamida	6	3	38

Second-stage model

For differentiation of the substance/substance group *Sulfacetamida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfacetamida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	166,21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfacetamida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfacetamida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfacetamida	11085910	20695	40	1402651
Caelo	Sulfacetamida	15445901	23251	40	20160126
Caelo	Sulfacetamida	15445901	23456	40	20160126
Caelo	Sulfacetamida	20002794001	25515	40	20201022
Euro OTC	Sulfacetamida	1312012-01	21633	60	20140117
Euro OTC	Sulfacetamida	1509018	21902	60	20150929*
Euro OTC	Sulfacetamida	2101027	25546	40	20210127*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Sulfacetamida*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sulfacetamida*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sulfacetamida	1702006	23157	40
Euro OTC	Sulfacetamida	1808035	24193	40
Euro OTC	Sulfacetamida	1907026	24804	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 184 spectra from 82 *Apo-Ident* customers from 43 batches from the substance/substance group *Sulfacetamida*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHC 12.08.13 EK9,31	Sulfacetamida	11085912	1
Apo-ident/Alliance	Sulfacetamida	1702006-02	1
Caelo	Sulfacetamida	10145802	1
Caelo	Sulfacetamida	10145811	1
Caelo	Sulfacetamida	11085909	1
Caelo	Sulfacetamida	11085911	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfacetamida	11085912	4
Caelo	Sulfacetamida	11085913	2
Caelo	Sulfacetamida	11085914	2
Caelo	Sulfacetamida	11095912	1
Caelo	Sulfacetamida	1509018-02	2
Caelo	Sulfacetamida	15445901	2
Caelo	Sulfacetamida	15445902	2
Caelo	Sulfacetamida	15445904	1
Caelo	Sulfacetamida	15445905	2
Caelo	Sulfacetamida	1702006-01	1
Caelo	Sulfacetamida	20002794001	1
Caelo	Sulfacetamida	20002794002	1
Caelo	Sulfacetamida	21003927003	1
Caesar & Loretz GmbH...	Sulfacetamida	20002794002	1
Caesar & Loretz GmbH	Sulfacetamida	15445902	2
Caesar & Loretz GmbH	Sulfacetamida	20002794001	2
Caesar & Loretz GmbH	Sulfacetamida	20002794002	4
Caesar & Loretz	Sulfacetamida	15445902	1
EuRho/Jenne	Sulfacetamida	2101027-01	1
EuRho/Noweda	Sulfacetamida	1702006-04	1
EuRho/Phönix	Sulfacetamida	1702006-02	1
EuRho	Sulfacetamida	210102701	1
Euro OTC	Sulfacetamida	1112032-01	3
Euro OTC	Sulfacetamida	1112032-02	4
Euro OTC	Sulfacetamida	1312012-01	4
Euro OTC	Sulfacetamida	1312012-02	2
Euro OTC	Sulfacetamida	1509018-01	5
Euro OTC	Sulfacetamida	1509018-02	5
Euro OTC	Sulfacetamida	1509018-03	3
Euro OTC	Sulfacetamida	1702006-01	3
Euro OTC	Sulfacetamida	1702006-02	3
Euro OTC	Sulfacetamida	170200604	1
Euro OTC	Sulfacetamida	1702006-04	3
Euro OTC	Sulfacetamida	1808035-01	2
Euro OTC	Sulfacetamida	1907026	1
Euro OTC	Sulfacetamida	190702601	3
Euro OTC	Sulfacetamida	1907026-01	33
Euro OTC	Sulfacetamida	2101027	1
Euro OTC	Sulfacetamida	2101027-01	24
Euro OTC	Sulfacetamida	5119E01073	1
Euro OTC	Sulfacetamida	AP210205-03	1
Euro OTC	Sulfacetamida	AP220721-02	1
EuroRho 24.05.2013 A...	Sulfacetamida	1112032-02	2
Gehe/EuRho	Sulfacetamida	2101027-02	1
Gehe	Sulfacetamida	11085904	1
Gehe	Sulfacetamida	1112032-01	4
Gehe	Sulfacetamida	1312012-01	2
Gehe	Sulfacetamida	1312012-02	1
Gehe	Sulfacetamida	1505025-01	1
Gehe	Sulfacetamida	190702601	1
Gehe	Sulfacetamida	1907026-01	2
Gehe	Sulfacetamida	2101027-01	1
Industrias GmbH / Ph	Sulfacetamida	64518	1
Katwijk Chemie B.V.	Sulfacetamida	15445902	3
Katwijk Chemie	Sulfacetamida	1702006-01	1
Noweda	Sulfacetamida	15445904	1
Noweda	Sulfacetamida	1702006-02	1
Noweda	Sulfacetamida	2101027-01	2
Noweda200002794001	Sulfacetamida	200002794001	1
Phoenix 17.02.2015	Sulfacetamida	1312012-02	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Sulfacetamida	15445904	1
Phönix 23.06.2014	Sulfacetamida	1312012-01	1
Phönix Gotha	Sulfacetamida	11085911	1
Phönix Gotha	Sulfacetamida	1312012-02	1
Phönix	Sulfacetamida	11085910	1
Phönix	Sulfacetamida	1509018-02	1
Phönix	Sulfacetamida	15445905	1
Phönix	Sulfacetamida	1907026-01	1
Spangropharm	Sulfacetamida	11085915	1

- 235 883 spectra from 1515 *Apo-Ident* customers from a total of 49 215 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfacetamida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfacetamida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	120	0	201 964
Type C	0	181	3	235 883

The substance/substance group *Sulfacetamida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.3696 % (> 96.7391 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20695	20695	0,00	357,73
21633	21902	9,82	362,73
21902	21902	0,00	363,74
23251	21902	9,64	355,15
23456	21902	7,80	358,55
25515	21902	12,37	357,54
25546	25546	0,00	359,69

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfadiazina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20753-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfadiazina; Sulfadiazinum

Special notes

When selecting the *Sulfadiazina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfadiazina	7	6	22

Second-stage model

For differentiation of the substance/substance group *Sulfadiazina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfadiazina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	215,07	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfadiazina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfadiazina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfadiazina	12164101	20753	40	1402053
Caelo	Sulfadiazina	13150011	21744	60	20130708
Caelo	Sulfadiazina	170566	23319	40	20170330*
Caelo	Sulfadiazina	17056602	23374	40	20170330
Caelo	Sulfadiazina	17056602	23447	40	20170330
Caelo	Sulfadiazina	191850	24735	40	20190730*
Caelo	Sulfadiazina	20000240002	25513	40	20200430
Caelo	Sulfadiazina	23003071	27233	40	20240220*
Caelo	Sulfadiazina	23003071	27233SI	20	20240220*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Sulfadiazina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 260 spectra of 8 reference samples from the substance/substance group *Sulfadiazina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfadiazina	172222	23630	30
Caelo	Sulfadiazina	190683	24523	40
Caelo	Sulfadiazina	21002176001	26412	40
Caelo	Sulfadiazina	24001426	27325	40
Fagron	Sulfadiazina	21G10-B22-216650	26061	40
Fagron	Sulfadiazina	23G05-B11-231251	27064	40
Fagron	Sulfadiazina	21G10-B22-216650	26061SI	10
Fagron	Sulfadiazina	23G05-B11-231251	27064SI	20

- 201 824 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 48 spectra from 23 *Apo-Ident* customers from 23 batches from the substance/substance group *Sulfadiazina*.

- Among them are spectra of independent samples from 22 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sulfadiazina	11194204	1
Caelo	Sulfadiazina	13150004	1
Caelo	Sulfadiazina	17358901	1
Caelo	Sulfadiazina	17358905	2
Caelo	Sulfadiazina	17358906	1
Caelo	Sulfadiazina	17358910	4
Caelo	Sulfadiazina	17358913	1
Caelo	Sulfadiazina	17358917	1
Caelo	Sulfadiazina	19068302	3
Caelo	Sulfadiazina	191850001	2
Caelo	Sulfadiazina	191850002	2
Caelo	Sulfadiazina	20000240002	4
Caelo	Sulfadiazina	20000240003	6
Caelo	Sulfadiazina	2000024002	2
Caelo	Sulfadiazina	200024003	1
Caelo	Sulfadiazina	20003569003	4
Caelo	Sulfadiazina	21002176001	1
Caelo	Sulfadiazina	21002176002	1
Caelo	Sulfadiazina	240002	1
Caesar & Loretz GmbH	Sulfadiazina	19068301	1
Caesar & Loretz GmbH	Sulfadiazina	19068302	1
Caesar & Loretz GmbH	Sulfadiazina	20000240005	2
Caesar & Loretz GmbH	Sulfadiazina	20000240006	1
Caesar & Loretz GmbH	Sulfadiazina	20003569002	1
Caesar & Loretz GmbH	Sulfadiazina	20003569003	3

- 236 019 spectra from 1515 *Apo-Ident* customers from a total of 49 235 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfadiazina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfadiazina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	260	0	201 824
Type C	0	48	0	236 019

The substance/substance group *Sulfadiazina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 87.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20753	20753	0,00	426,89
21744	23319	7,00	431,46
23319	23319	0,00	431,44
23374	23319	6,08	430,23
23447	23319	4,74	431,09
24735	24735	0,00	432,03
25513	20753	8,58	430,93
27233	27233	0,00	429,67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de anfetamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20299-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de anfetamina; Amfetamini sulfas; Anfetamina, sulfato

Special notes

When selecting the *Sulfato de anfetamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de anfetamina	6	2	93

Second-stage model

For differentiation of the substance/substance group *Sulfato de anfetamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de anfetamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de dexanfetamina	67,58	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de anfetamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de anfetamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de anfetamina	13344603	21132	40	0814J-03361
Caelo	Sulfato de anfetamina	13344603	21132SI	60	0814J-03361
Caelo	Sulfato de anfetamina	16153902	23461	40	2017A-03361
Fagron	Sulfato de anfetamina	13G08-N11	21130	40	0814K-03361
Fagron	Sulfato de anfetamina	13G08-N11	21130SI	60	0814K-03361
Fagron	Sulfato de anfetamina	15L01-B05-315291	22430	60	1316Q-03361
Fagron	Sulfato de anfetamina	15L01-B05-315291	22430SI	60	1316Q-03361
Th. Geyer	Sulfato de anfetamina	67002	21134	40	0814I-03361
Th. Geyer	Sulfato de anfetamina	67002	21134SI	60	0814I-03361
Th. Geyer	Sulfato de anfetamina	067043	23459	40	2017C-03361

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 500 spectra of 10 reference samples from the substance/substance group *Sulfato de anfetamina*. These samples are listed above in the *calibration samples* section. The reference samples come

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

from 6 different batches.

- 152 462 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Sulfato de anfetamina*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de anfetamina	18186907	24646	40
Fagron	Sulfato de anfetamina	16A29-B03-324577	23460	40
Caelo	Sulfato de anfetamina	16153902	23461SI†	40
Caelo	Sulfato de anfetamina	18186907	24646SI	40
Fagron	Sulfato de anfetamina	16A29-B03-324577	23460SI	40
Th. Geyer	Sulfato de anfetamina	067043	23459SI†	40

- 201 844 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 451 spectra from 171 *Apo-Ident* customers from 102 batches from the substance/substance group *Sulfato de anfetamina*.

- Among them are spectra of independent samples from 92 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de anfetamina	22I08-F02-383423	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Alkoholvertrieb Süd	Sulfato de anfetamina	67043	2
Anzag/Th.Gyer GmbH	Sulfato de anfetamina	67043	1
BLS /Gehe	Sulfato de anfetamina	70325	2
BLS Analytik GmbH/ S...	Sulfato de anfetamina	70325	5
BLS Analytik GmbH	Sulfato de anfetamina	70325	5
BLS Analytik	Sulfato de anfetamina	67043	1
BLS Analytik	Sulfato de anfetamina	70325	1
BLS/Jenne	Sulfato de anfetamina	70325	4
BLS/Noweda	Sulfato de anfetamina	67043	1
BLS-Analytik GmbH/AHD	Sulfato de anfetamina	70325	1
BLS-Analytik GmbH	Sulfato de anfetamina	70325	1
BLS-Analytik/Phönix	Sulfato de anfetamina	70325	1
Bombastus	Sulfato de anfetamina	C18H28N2O4S	1
Caelo	Sulfato de anfetamina	12B06-N013	1
Caelo	Sulfato de anfetamina	12I24-N03	1
Caelo	Sulfato de anfetamina	13344609	1
Caelo	Sulfato de anfetamina	13G08-N11	2
Caelo	Sulfato de anfetamina	15193204	3
Caelo	Sulfato de anfetamina	15L01-B05	2
Caelo	Sulfato de anfetamina	15L01-B05-315291	2
Caelo	Sulfato de anfetamina	16143001	1
Caelo	Sulfato de anfetamina	16153902	1
Caelo	Sulfato de anfetamina	16153903	4
Caelo	Sulfato de anfetamina	16153905	3
Caelo	Sulfato de anfetamina	16153909	1
Caelo	Sulfato de anfetamina	16A29-B03-318744	1
Caelo	Sulfato de anfetamina	17K03-B01	1
Caelo	Sulfato de anfetamina	1807171	1
Caelo	Sulfato de anfetamina	18186903	1
Caelo	Sulfato de anfetamina	200004272001	1
Caelo	Sulfato de anfetamina	200004272009	1
Caelo	Sulfato de anfetamina	20004272001	3
Caelo	Sulfato de anfetamina	20004272011	2
Caelo	Sulfato de anfetamina	2004272001	1
Caelo	Sulfato de anfetamina	22003072004	1
Caelo	Sulfato de anfetamina	67043	11
Caelo	Sulfato de anfetamina	70325	11
Caelo	Sulfato de anfetamina	lot067002	1
Caesar & Loretz GmbH/Gehe	Sulfato de anfetamina	22003072003	3
Caesar & Loretz GmbH	Sulfato de anfetamina	16153901	1
Caesar & Loretz GmbH	Sulfato de anfetamina	16153905	1
Caesar & Loretz GmbH	Sulfato de anfetamina	20004272001	2
Caesar & Loretz GmbH	Sulfato de anfetamina	20004272002	2
Caesar & Loretz GmbH	Sulfato de anfetamina	22003072002	1
Euro OTC	Sulfato de anfetamina	16A29-B03-324578	1
Euro OTC	Sulfato de anfetamina	67043	5
Euro OTC	Sulfato de anfetamina	70325	3
Euro/Noweda	Sulfato de anfetamina	70325	1
Fagron	Sulfato de anfetamina	11/01-N01	1
Fagron	Sulfato de anfetamina	1117I-03361	1
Fagron	Sulfato de anfetamina	11D04-N13	1
Fagron	Sulfato de anfetamina	12/24N-03	1
Fagron	Sulfato de anfetamina	12B06-N13	2
Fagron	Sulfato de anfetamina	12E11-N06	2
Fagron	Sulfato de anfetamina	13B11-N04	1
Fagron	Sulfato de anfetamina	13D09-N03	1
Fagron	Sulfato de anfetamina	13G08-N11	1
Fagron	Sulfato de anfetamina	13J18B40	1
Fagron	Sulfato de anfetamina	13J18-B40	1
Fagron	Sulfato de anfetamina	13J18-B40-290538	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de anfetamina	14E19-B09	2
Fagron	Sulfato de anfetamina	14E19-B09-294572	1
Fagron	Sulfato de anfetamina	14E19-B09-304502	2
Fagron	Sulfato de anfetamina	15L01-B05	1
Fagron	Sulfato de anfetamina	15L01-B05-315290	1
Fagron	Sulfato de anfetamina	15L01-B05-315291	4
Fagron	Sulfato de anfetamina	15l01-b05-315292	1
Fagron	Sulfato de anfetamina	15L01-B05-315292	7
Fagron	Sulfato de anfetamina	16A29_B03_318744	1
Fagron	Sulfato de anfetamina	16A29-B03	11
Fagron	Sulfato de anfetamina	16A29-B03-318743	6
Fagron	Sulfato de anfetamina	16a29-b03-318744	2
Fagron	Sulfato de anfetamina	16A29B03318744	1
Fagron	Sulfato de anfetamina	16a29-B03-319156	1
Fagron	Sulfato de anfetamina	16A29-B03-324578	2
Fagron	Sulfato de anfetamina	16A29-B03-328317	4
Fagron	Sulfato de anfetamina	16A29-B03-328318	1
Fagron	Sulfato de anfetamina	16K08-B04	1
Fagron	Sulfato de anfetamina	16K08-B04-336361	2
Fagron	Sulfato de anfetamina	16K08B04336362	1
Fagron	Sulfato de anfetamina	16K08-B04-336362	1
Fagron	Sulfato de anfetamina	17K03-B01-344122	3
Fagron	Sulfato de anfetamina	19H05-B01	1
Fagron	Sulfato de anfetamina	19H05-B01-3633407	1
Fagron	Sulfato de anfetamina	19H05-B01-363345	2
Fagron	Sulfato de anfetamina	19H05-B01-363346	4
Fagron	Sulfato de anfetamina	19H05-B01-363347	1
Fagron	Sulfato de anfetamina	19H05-B01-364791	1
Fagron	Sulfato de anfetamina	19h05b01365581	1
Fagron	Sulfato de anfetamina	19H05-B01-365581	2
Fagron	Sulfato de anfetamina	19H05-B01-365582	3
Fagron	Sulfato de anfetamina	20I18-F06	2
Fagron	Sulfato de anfetamina	2213Q-03361	1
Fagron	Sulfato de anfetamina	315291	1
Fagron	Sulfato de anfetamina	324577	2
Fagron	Sulfato de anfetamina	67043	1
Fagron	Sulfato de anfetamina	70325	3
Fagron	Sulfato de anfetamina	78012	1
Fagron	Sulfato de anfetamina	88689	2
Fagron	Sulfato de anfetamina	96200	2
Fagron	Sulfato de anfetamina	B01_3655801	1
Fagron	Sulfato de anfetamina	F001287	1
Gatt Koller/Herba	Sulfato de anfetamina	942/03130814	1
Gatt-Koller	Sulfato de anfetamina		1
Gatt-Koller	Sulfato de anfetamina	22J01850	1
Gehe	Sulfato de anfetamina	13B11-N04	1
Hedinger	Sulfato de anfetamina	67002	1
Kehr	Sulfato de anfetamina	67043	1
L30	Sulfato de anfetamina	16A29-B03-328317	1
Noweda 7.8.19	Sulfato de anfetamina	70325P-190808-1	1
Noweda	Sulfato de anfetamina	16A29-B03-318744	2
Noweda	Sulfato de anfetamina	16A29-B03-324578	1
Phoenix	Sulfato de anfetamina	16A29-B03-328317	1
Phönix	Sulfato de anfetamina	13B11N04	1
Phönix	Sulfato de anfetamina	16a29-b03-328317	1
Phönix	Sulfato de anfetamina	16A29-B03-328317	1
Phönix	Sulfato de anfetamina	19H05-B01-363345	2
Phönix	Sulfato de anfetamina	70325	4
Sanacorp	Sulfato de anfetamina	12/24-N03	1
Sanacorp	Sulfato de anfetamina	67043	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Th. Geyer	Sulfato de anfetamina		2
Th. Geyer	Sulfato de anfetamina	20170808-03361	1
Th. Geyer	Sulfato de anfetamina	21082013B	1
Th. Geyer	Sulfato de anfetamina	57043	1
Th. Geyer	Sulfato de anfetamina	618E-03361	1
Th. Geyer	Sulfato de anfetamina	67002	48
Th. Geyer	Sulfato de anfetamina	6703	1
Th. Geyer	Sulfato de anfetamina	67043	70
Th. Geyer	Sulfato de anfetamina	67043P-180924-1	1
Th. Geyer	Sulfato de anfetamina	70325	75
Th. Geyer	Sulfato de anfetamina	70325P-190404-1	1
Th. Geyer	Sulfato de anfetamina	70525	1
Th. Geyer	Sulfato de anfetamina	LOT067043	1
Th. Geyer	Sulfato de anfetamina	LOT070325	2
Th. Geyer	Sulfato de anfetamina	PH10051	3
Th.Gever über Phoenix	Sulfato de anfetamina	67002	2
TH.Grever GmbH/Sanacorp	Sulfato de anfetamina	70325	1
Th.Greyer/Gehe	Sulfato de anfetamina	67043	2
Th.Greyer/Krieger	Sulfato de anfetamina	70325	4
Th.Greyer/Sanacorp	Sulfato de anfetamina	70325	1
Th.Gryer Gmbh	Sulfato de anfetamina	70325	1

- 235 616 spectra from 1515 *Apo-Ident* customers from a total of 49 157 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de anfetamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de anfetamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	500	0	152 462
Type B	0	240	0	201 844
Type C	0	443	8	235 616

The substance/substance group *Sulfato de anfetamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.2262 % (> 97.5610 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21130	21130	0,00	83,48
21132	21132	0,00	83,20
21134	21134	0,00	82,99
22430	22430	0,00	86,31
23459	23459	0,00	88,80
23461	23461	0,00	82,66

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de atropina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20653-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de atropina; Atropina, sulfato; Atropini sulfas

Special notes

When selecting the *Sulfato de atropina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de atropina	7	6	32

Second-stage model

For differentiation of the substance/substance group *Sulfato de atropina* the following second-stage model is used:

- Submodelo 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de atropina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	79,92	–
⋮	⋮	⋮
Furoato de mometasona	>50	43,26
Sorbato de potássio	>50	110,83
Cloridrato de propranolol	>50	149,70
Citrato monobásico de magnésio, hid…	>50	169,38
Hidrocortisona	>50	239,00
Quinolina amarela	>50	251,76
Sacarina sódica	>50	279,62
Fenitoína	>50	302,00
Escina, hidrossolúvel	>50	436,09
Orotato de cálcio di-hidratado	>50	481,80

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de atropina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de atropina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de atropina	11180602	20653	30	1405538
Caelo	Sulfato de atropina	13173808	21088	40	1403483
Caelo	Sulfato de atropina	13357405	21551	50	1504594
Caelo	Sulfato de atropina	14336806	21719	60	1510209
Caelo	Sulfato de atropina	14336806	21719SI	60	1510209
Caelo	Sulfato de atropina	15301601	21920	60	20150930
Caelo	Sulfato de atropina	15301601	21920SI	60	20150930
Caelo	Sulfato de atropina	172732	23682	40	20171020*
Fagron	Sulfato de atropina	16G20-B06-328437	22932	40	20160823

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 9 reference samples from the substance/substance group *Sulfato de atropina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 550 spectra of 14 reference samples from the substance/substance group *Sulfato de atropina*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de atropina	16326802	22952	40
Caelo	Sulfato de atropina	170264	23367	40
Caelo	Sulfato de atropina	22002311	26353	40
Caelo	Sulfato de atropina	23002005	26949	40
Fagron	Sulfato de atropina	22E05-B03-220032	26298	40
Fagron	Sulfato de atropina	23J24-B05-233615	27241	40
Caelo	Sulfato de atropina	16326802	22952SI	40
Caelo	Sulfato de atropina	170264	23367SI	40
Caelo	Sulfato de atropina	172732	23682SI†	30
Caelo	Sulfato de atropina	22002311	26353SI	40
Caelo	Sulfato de atropina	23002005	26949SI	40
Fagron	Sulfato de atropina	16G20-B06-328437	22932SI†	40
Fagron	Sulfato de atropina	22E05-B03-220032	26298SI	40
Fagron	Sulfato de atropina	23J24-B05-233615	27241SI	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 534 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 87 spectra from 65 *Apo-Ident* customers from 33 batches from the substance/substance group *Sulfato de atropina*.
- Among them are spectra of independent samples from 32 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de atropina	23000208003	7
	Sulfato de atropina	23002005004	2
	Sulfato de atropina	23J24-B05-233615	1
AHD	Sulfato de atropina	23000208003	1
ATS 200005	Sulfato de atropina	21000738004	1
Caelo	Sulfato de atropina	13173809	1
Caelo	Sulfato de atropina	13357403	1
Caelo	Sulfato de atropina	13357405	1
Caelo	Sulfato de atropina	14336807	1
Caelo	Sulfato de atropina	15115201	3
Caelo	Sulfato de atropina	16326802	3
Caelo	Sulfato de atropina	16c15b03-319166	1
Caelo	Sulfato de atropina	17273202	1
Caelo	Sulfato de atropina	18099107	1
Caelo	Sulfato de atropina	18099111	3
Caelo	Sulfato de atropina	18276501	1
Caelo	Sulfato de atropina	18276510	2
Caelo	Sulfato de atropina	192937003	1
Caelo	Sulfato de atropina	192937007	4
Caelo	Sulfato de atropina	21000146001	1
Caelo	Sulfato de atropina	21000738001	7
Caelo	Sulfato de atropina	21000738004	4
Caelo	Sulfato de atropina	21000738007	2
Caelo	Sulfato de atropina	22000757003	2
Caelo	Sulfato de atropina	22002311003	3
Caelo	Sulfato de atropina	70446207	1
Caelo	Sulfato de atropina	738001	1
Caesar & Loretz GmbH...	Sulfato de atropina	18276501	1
Caesar & Loretz GmbH...	Sulfato de atropina	192937007	1
Caesar & Loretz GmbH...	Sulfato de atropina	21000738004	1
Caesar & Loretz GmbH...	Sulfato de atropina	18099111	1
Caesar & Loretz GmbH...	Sulfato de atropina	22000757003	1
Caesar & Loretz GmbH...	Sulfato de atropina	182765	1
Caesar & Loretz GmbH...	Sulfato de atropina	192937	1
Caesar & Loretz GmbH...	Sulfato de atropina	192937007	1
Caesar & Loretz GmbH	Sulfato de atropina	192937003	2
Caesar & Loretz GmbH	Sulfato de atropina	192937007	4
Caesar & Loretz GmbH	Sulfato de atropina	21000738001	2
Caesar & Loretz GmbH	Sulfato de atropina	22000757003	4
fargon	Sulfato de atropina	13K01-N01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Sulfato de atropina	16326802	1
GEHE	Sulfato de atropina	17273202	1
Noweda	Sulfato de atropina	12250403	1
Noweda	Sulfato de atropina	18276510	1
Noweda	Sulfato de atropina	23000208002	1
Parthe Apotheke	Sulfato de atropina	120/20	1
Parthe Apotheke	Sulfato de atropina	50/21	1
Phönix	Sulfato de atropina	15301607	1
Sanacorp	Sulfato de atropina	23000208003	1

- 235 980 spectra from 1515 *Apo-Ident* customers from a total of 49 225 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de atropina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de atropina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	550	0	201 534
Type C	0	84	3	235 980

The substance/substance group *Sulfato de atropina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9091 %)
Type C	100.0000 % (> 99.9007 %)	96.5517 % (> 93.1034 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20653	20653	0,00	214,92
21088	21088	0,00	202,59
21551	21551	0,00	212,71
21719	21719	0,00	159,45
21920	21719	21,31	178,72
22932	21088	17,92	196,43
23682	23682	0,00	162,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de colistina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20318-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de colistina; Colistina, sulfato; Colistini sulfas

Special notes

When selecting the *Sulfato de colistina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de colistina	10	10	14

Second-stage model

For differentiation of the substance/substance group *Sulfato de colistina* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de colistina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	30,16	19,07
Bacitracina	37,51	13,73
Pantotenato de cálcio	73,77	37,92
⋮	⋮	⋮
Anfotericina B	>50	47,48
Vitamina E acetato pó 50%	>50	53,69
Cianocobalamina	>50	56,43
Riboflavina	>50	65,17
Levedura de selênio	>50	65,82
Metilcobalamina	>50	67,50
Nistatina	>50	70,19
Gelatina, branca	>50	73,76
Estradiol hemi-hidratado	>50	75,59
Estriol	>50	77,96
Triancinolona	>50	87,83
Glicerofosfato de cálcio	>50	102,98
Carmelose sódica	>50	129,47
Bromidrato de hioscina	>50	158,25
SyrSpend® SF Alka	>50	199,28
Tosilcloramida sódica	>50	202,04
Amido de arroz	>50	230,94
SyrSpend® SF pH4 neo	>50	288,81
Ácido oxálico	>50	315,11
Goma arábica, dispersão seca	>50	324,46
Amido de milho	>50	326,55
SyrSpend® SF pH4	>50	402,15
Maltodextrina	>50	453,41
Fécula de batata	>50	463,39
Amido de trigo	>50	469,46
Frutose	>50	552,70

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de colistina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de colistina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Sulfato de colistina	APKB-CS-1602026C	22974	40	20160418
Audor Pharma	Sulfato de colistina	APKB-CS-1602026C	23027	40	20160418
Euro OTC	Sulfato de colistina	1406001-01	21619	60	1508600
Euro OTC	Sulfato de colistina	1507044	21852	60	20150817*
Euro OTC	Sulfato de colistina	1602021	22371	60	20160307*
Euro OTC	Sulfato de colistina	1606008	22695	40	20160704*
Euro OTC	Sulfato de colistina	2009035	25431	40	20200930*
Fagron	Sulfato de colistina	13G05-N01	20915	40	20130719
Fagron	Sulfato de colistina	13G05-N01	21209	40	20130719
Fagron	Sulfato de colistina	14E02-B03	21346	40	1501654
Fagron	Sulfato de colistina	16F03-B01-324216	22973	40	20160706
Fagron	Sulfato de colistina	20F18-B04-201974	25667	50	20200706

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 12 reference samples from the substance/substance group *Sulfato de colistina*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 412 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 465 spectra of 13 reference samples from the substance/substance group *Sulfato de colistina*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Sulfato de colistina	APKB-CS-1603034C	23026	40
Euro OTC	Sulfato de colistina	1406002-01	21700	45
Euro OTC	Sulfato de colistina	1709009	23616	40
Euro OTC	Sulfato de colistina	1710041	23866	40
Euro OTC	Sulfato de colistina	1905016	24769	40
Euro OTC	Sulfato de colistina	1908007	24836	40
Euro OTC	Sulfato de colistina	2001039	25087	40
Euro OTC	Sulfato de colistina	2301012	26653	40
Fagron	Sulfato de colistina	22B14-B10-219015	26182	40
Fagron	Sulfato de colistina	23D12-B10-230780	27382	40
Euro OTC	Sulfato de colistina	2301012	26653SI	20
Fagron	Sulfato de colistina	22B14-B10-219015	26182SI	20
Fagron	Sulfato de colistina	23D12-B10-230780	27382SI	20

- 201 619 spectra from a total of 4035 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 8 *Apo-Ident* customers from 16 batches from the substance/substance group *Sulfato de colistina*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Audor Pharma	Sulfato de colistina	APKB-CS-1601026C	1
Audor Pharma	Sulfato de colistina	APKB-CS-1603034C	2
Audor Pharma	Sulfato de colistina	APKB-CS-1610012C	1
Caelo	Sulfato de colistina	1602021-01	1
Euro OTC	Sulfato de colistina	1507044-01	1
Fagron	Sulfato de colistina	15E15-B01-315340	1
Fagron	Sulfato de colistina	16F03-B01	1
Fagron	Sulfato de colistina	16F03-B01_322758	1
Fagron	Sulfato de colistina	16f03-b01-324216	1
Fagron	Sulfato de colistina	16F03-B01-324216	1
Fagron	Sulfato de colistina	16J03-B10-330367	1
Fagron	Sulfato de colistina	17E09-B04-342085	1
Fagron	Sulfato de colistina	17j24-b03-342638	1
Fagron	Sulfato de colistina	20K06-B03-202435	2
Fagron	Sulfato de colistina	21G20_B09213652	1
Fagron	Sulfato de colistina	21G20-B08-215430	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Sulfato de colistina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de colistina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	512	38	152 412
Type B	0	465	0	201 619
Type C	0	18	0	236 049

The substance/substance group *Sulfato de colistina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	93.0909 % (> 92.5455 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7097 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20915	21619	8,77	49,67
21209	21619	8,04	45,61
21346	21346	0,00	37,09
21619	21619	0,00	46,23
21852	21852	0,00	37,27
22371	22371	0,00	53,81
22695	22695	0,00	38,27
22973	21852	3,20	36,84
22974	21852	16,60	36,05
23027	21346	17,16	35,74
25431	25431	0,00	59,54
25667	22695	23,61	37,51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de condroitina sódico**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	24283-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de condroitina sódico

Special notes

When selecting the *Sulfato de condroitina sódico* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de condroitina sódico	2	1	0

Second-stage model

For differentiation of the substance/substance group *Sulfato de condroitina sódico* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de condroitina sódico* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	59,57	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de condroitina sódico* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de condroitina sódico*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Yino Pharma	Sulfato de condroitina sódico	YN010511806006	24284	40	20180912*
Yino Pharma	Sulfato de condroitina sódico	YN010511805005	24285	40	20180912*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Sulfato de condroitina sódico*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Sulfato de condroitina sódico*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Yino Pharma	Sulfato de condroitina sódico	YN010511806007	24283	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sulfato de condroitina sódico*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de condroitina sódico* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de condroitina sódico* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Sulfato de condroitina sódico* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24284	24284	0,00	75,84
24285	24285	0,00	70,59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de dexanfetamina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21154-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de dexanfetamina; Dexamfetamini sulfas; Dexanfetamina, sulfato

Special notes

When selecting the *Sulfato de dexanfetamina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de dexanfetamina	3	1	22

Second-stage model

For differentiation of the substance/substance group *Sulfato de dexanfetamina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de dexanfetamina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de anfetamina	61,19	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de dexanfetamina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de dexanfetamina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulfato de dexanfetamina	13I23-N01	21154	40	0814M-03582
Fagron	Sulfato de dexanfetamina	13I23-N01	21154SI	60	0814M-03582
Fagron	Sulfato de dexanfetamina	15H06-B04-313862	22426	60	1316Q-03582
Fagron	Sulfato de dexanfetamina	16D20-B01-321049	23474	40	2017B-03582

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Sulfato de dexanfetamina*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 762 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 4 reference samples from the substance/substance group *Sulfato de dexanfetamina*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Sulfato de dexanfetamina	16F09-B02-328352	23475	40
Fagron	Sulfato de dexanfetamina	15H06-B04-313862	22426SI†	60
Fagron	Sulfato de dexanfetamina	16D20-B01-321049	23474SI†	40
Fagron	Sulfato de dexanfetamina	16F09-B02-328352	23475SI	40

- 201 904 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 39 spectra from 17 *Apo-Ident* customers from 22 batches from the substance/substance group *Sulfato de dexanfetamina*.
- Among them are spectra of independent samples from 22 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de dexanfetamina	22A18-F01-383287	2
Caelo	Sulfato de dexanfetamina	C9H13N14	1
Fagron	Sulfato de dexanfetamina	11F29-N01	1
Fagron	Sulfato de dexanfetamina	15H06-B04-313861	1
Fagron	Sulfato de dexanfetamina	16F09-B02-328352	1
Fagron	Sulfato de dexanfetamina	17B019-B02-339689	1
Fagron	Sulfato de dexanfetamina	17B09-B02	2
Fagron	Sulfato de dexanfetamina	17B09-B02-339689	4

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de dexanfetamina	17B09-B02-339690	1
Fagron	Sulfato de dexanfetamina	19D12-B50	2
Fagron	Sulfato de dexanfetamina	19D12-B50-363246	3
Fagron	Sulfato de dexanfetamina	19D12-B50-363247	6
Fagron	Sulfato de dexanfetamina	20D10-F02	3
Fagron	Sulfato de dexanfetamina	20D10-F02_370503	1
Fagron	Sulfato de dexanfetamina	20D10-F02-370502	1
Fagron	Sulfato de dexanfetamina	20D10-F02-370503	1
Fagron	Sulfato de dexanfetamina	22A18-F01-383285	1
Fagron	Sulfato de dexanfetamina	B50-3632406	2
Fagron	Sulfato de dexanfetamina	F01-3764108	1
Fagron	Sulfato de dexanfetamina	F02-3705003	2
Fargon/ Phönix	Sulfato de dexanfetamina	F000876	1
Fargon/Gehe	Sulfato de dexanfetamina	15H06-B04	1

- 236 028 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de dexanfetamina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de dexanfetamina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	180	0	201 904
Type C	0	39	0	236 028

The substance/substance group *Sulfato de dexanfetamina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.6154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21154	21154	0,00	83,89
22426	22426	0,00	85,42
23474	23474	0,00	94,51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de gentamicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20640-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de gentamicina; Gentamicina, sulfato; Gentamicini sulfas

Special notes

When selecting the *Sulfato de gentamicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de gentamicina	17	9	358

Second-stage model

For differentiation of the substance/substance group *Sulfato de gentamicina* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de gentamicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	46,53	–
Sulfato de polimixina B	48,85	–
Fosfato sódico de riboflavina hidratado	51,77	32,87
⋮	⋮	⋮
Fosfato de Mg-Ca-K-colamina	>50	36,72
Citrato de magnésio	>50	62,40
Sulfato de neomicina	>50	74,18
Carbômero	>50	77,76
Gluconato de zinco	>50	103,21
Sulfato de tobramicina	>50	126,45
Tetraborato de sódio	>50	262,45
Finasterida	>50	1065,07

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de gentamicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de gentamicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de gentamicina	13205003	21580	60	20130723
Caelo	Sulfato de gentamicina	14353504	22604	40	20150119
Caelo	Sulfato de gentamicina	192564	25201	40	20191218*
Caelo	Sulfato de gentamicina	192564	25201SI	40	20191218*
Caelo	Sulfato de gentamicina	20003226	25638	40	20201029*
Caelo	Sulfato de gentamicina	20003226	25638SI	40	20201029*
Euro OTC	Sulfato de gentamicina	1305047-01	21081	30	20130919
Euro OTC	Sulfato de gentamicina	1305047-03	21582	60	1411076
Euro OTC	Sulfato de gentamicina	1305047-03	21697	45	AR-15-FG-012403-01
Euro OTC	Sulfato de gentamicina	1506016	21837	60	0000010321

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Sulfato de gentamicina	1610036	22857	40	20161124*
Euro OTC	Sulfato de gentamicina	1610036-01	23782	40	1804343
Euro OTC	Sulfato de gentamicina	1711025	23882	40	20171206*
Euro OTC	Sulfato de gentamicina	1711025	23882SI	40	20171206*
Euro OTC	Sulfato de gentamicina	1907036	24866	40	20190823*
Euro OTC	Sulfato de gentamicina	2003058	25252	40	20200603*
Euro OTC	Sulfato de gentamicina	2003058	25252SI	40	20200603*
Fagron	Sulfato de gentamicina	12B21-N02	20661	40	1411075
Fagron	Sulfato de gentamicina	13I19-B05-286565	21578	60	20121214
Fagron	Sulfato de gentamicina	14E08-B03-294848	21684	60	20140616
Fagron	Sulfato de gentamicina	16B29-B01-328731	23210	40	20160411
Fagron	Sulfato de gentamicina	19G17-B05-193462	25180	40	20190805
Fagron	Sulfato de gentamicina	19G17-B05-193462	25180SI	40	20190805

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1015 spectra of 23 reference samples from the substance/substance group *Sulfato de gentamicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 17 different batches.

- 151 947 spectra from a total of 2825 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 950 spectra of 21 reference samples from the substance/substance group *Sulfato de gentamicina*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de gentamicina	170996	23335	40
Caelo	Sulfato de gentamicina	183001	24357	40
Caelo	Sulfato de gentamicina	23001024	27128	40
Euro OTC	Sulfato de gentamicina	1604054	22568	40
Euro OTC	Sulfato de gentamicina	1808013	24300	40
Euro OTC	Sulfato de gentamicina	2107013	25825	50
Euro OTC	Sulfato de gentamicina	2203032	26083	40
Euro OTC	Sulfato de gentamicina	2210010	26434	40
Fagron	Sulfato de gentamicina	22C17-B10-218675	26181	40
Caelo	Sulfato de gentamicina	13205003	21580SI†	60
Caelo	Sulfato de gentamicina	183001	24357SI	40
Caelo	Sulfato de gentamicina	23001024	27128SI	40
Euro OTC	Sulfato de gentamicina	1506016	21837SI†	60
Euro OTC	Sulfato de gentamicina	1808013	24300SI	40
Euro OTC	Sulfato de gentamicina	1907036	24866SI†	40
Euro OTC	Sulfato de gentamicina	2107013	25825SI	50
Euro OTC	Sulfato de gentamicina	2203032	26083SI	50
Euro OTC	Sulfato de gentamicina	2210010	26434SI	40
Fagron	Sulfato de gentamicina	13I19-B05-286565	21578SI†	60
Fagron	Sulfato de gentamicina	14E08-B03-294848	21684SI†	60
Fagron	Sulfato de gentamicina	22C17-B10-218675	26181SI	40

- 201 134 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2537 spectra from 961 *Apo-Ident* customers from 384 batches from the substance/substance group *Sulfato de gentamicina*.

- Among them are spectra of independent samples from 355 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de gentamicina	1610038-01	1
	Sulfato de gentamicina	20004483009	1
	Sulfato de gentamicina	20004483012	1
	Sulfato de gentamicina	2107013-02	2
	Sulfato de gentamicina	210920013	1
	Sulfato de gentamicina	2200075012	1
	Sulfato de gentamicina	22000754001	3
	Sulfato de gentamicina	22000754003	8
	Sulfato de gentamicina	22000754006	4
	Sulfato de gentamicina	22000754011	2
	Sulfato de gentamicina	22000754012	6
	Sulfato de gentamicina	22000754013	5
	Sulfato de gentamicina	2203032-01	3
	Sulfato de gentamicina	2210010-01	4

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Sulfato de gentamicina	2210010-02	2
	Sulfato de gentamicina	2210010-03	1
	Sulfato de gentamicina	22C17-B010-223074	1
	Sulfato de gentamicina	22C17-B10	1
	Sulfato de gentamicina	22c17-b10-223074	1
	Sulfato de gentamicina	22F28-B02-233049	1
	Sulfato de gentamicina	22I14-B01-227901	1
	Sulfato de gentamicina	23001024001	3
	Sulfato de gentamicina	23001024004	9
	Sulfato de gentamicina	23001024005	1
	Sulfato de gentamicina	23G05-B07-236824	1
AHD /Pharmachem Pößneck	Sulfato de gentamicina	1506016-02	1
AHD 29.10.14 EK6,12	Sulfato de gentamicina	13205004	1
AHD Lamotte GmbH	Sulfato de gentamicina	1604054-02	1
AHD	Sulfato de gentamicina	13205005	2
AHD	Sulfato de gentamicina	22000754003	1
AHD	Sulfato de gentamicina	22000754012	1
AHD	Sulfato de gentamicina	22000754013	1
AHD	Sulfato de gentamicina	23001024001	1
ALH	Sulfato de gentamicina	15258813	1
ALH	Sulfato de gentamicina	15258816	1
Alliance Healtcare	Sulfato de gentamicina	2003058-01	3
Alliance Healthcare	Sulfato de gentamicina	12G04-N16	1
Anzag	Sulfato de gentamicina	12146602	1
Anzag	Sulfato de gentamicina	1305047-03	1
Anzag	Sulfato de gentamicina	1407024-01	1
Anzag	Sulfato de gentamicina	17K16-B09-343323	1
Apo Ident/ Noweda	Sulfato de gentamicina	1711025	1
Apotheke	Sulfato de gentamicina	2003058-02	2
Audor Pharma	Sulfato de gentamicina	1604054-01	1
Bombastus	Sulfato de gentamicina	1205021-01	1
Bombastus	Sulfato de gentamicina	13024-N05	1
Bombastus	Sulfato de gentamicina	17358616	1
Bombastus	Sulfato de gentamicina	700175	1
Caelo	Sulfato de gentamicina		3
Caelo	Sulfato de gentamicina	10(18300112)	1
Caelo	Sulfato de gentamicina	100017814	1
Caelo	Sulfato de gentamicina	1106016-01	1
Caelo	Sulfato de gentamicina	1106016-03	1
Caelo	Sulfato de gentamicina	11113303	2
Caelo	Sulfato de gentamicina	11113304	1
Caelo	Sulfato de gentamicina	11113308	4
Caelo	Sulfato de gentamicina	115258818	1
Caelo	Sulfato de gentamicina	12011801	1
Caelo	Sulfato de gentamicina	1205021-01	1
Caelo	Sulfato de gentamicina	1205021-02	2
Caelo	Sulfato de gentamicina	12146602	7
Caelo	Sulfato de gentamicina	12146604	6
Caelo	Sulfato de gentamicina	12146605	4
Caelo	Sulfato de gentamicina	12146611	11
Caelo	Sulfato de gentamicina	12146612	2
Caelo	Sulfato de gentamicina	12163204	4
Caelo	Sulfato de gentamicina	12163206	1
Caelo	Sulfato de gentamicina	12163207	3
Caelo	Sulfato de gentamicina	12163209	1
Caelo	Sulfato de gentamicina	12258813	1
Caelo	Sulfato de gentamicina	1260417	1
Caelo	Sulfato de gentamicina	12G04-N16	2
Caelo	Sulfato de gentamicina	130205005	1
Caelo	Sulfato de gentamicina	1305047-03	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de gentamicina	1305047-03(2mal)	1
Caelo	Sulfato de gentamicina	13091207	1
Caelo	Sulfato de gentamicina	13189602	5
Caelo	Sulfato de gentamicina	13189603	3
Caelo	Sulfato de gentamicina	13189606	6
Caelo	Sulfato de gentamicina	13189607	11
Caelo	Sulfato de gentamicina	13189608	2
Caelo	Sulfato de gentamicina	13189611	10
Caelo	Sulfato de gentamicina	13189612	13
Caelo	Sulfato de gentamicina	13189613	1
Caelo	Sulfato de gentamicina	13189614	2
Caelo	Sulfato de gentamicina	13205003	10
Caelo	Sulfato de gentamicina	13205004	2
Caelo	Sulfato de gentamicina	13205005	17
Caelo	Sulfato de gentamicina	13205006	6
Caelo	Sulfato de gentamicina	13205007	2
Caelo	Sulfato de gentamicina	13D24-N05	1
Caelo	Sulfato de gentamicina	13I19-B05-286565	1
Caelo	Sulfato de gentamicina	14081307	1
Caelo	Sulfato de gentamicina	1435303	2
Caelo	Sulfato de gentamicina	143533504	1
Caelo	Sulfato de gentamicina	143535	1
Caelo	Sulfato de gentamicina	14353502	3
Caelo	Sulfato de gentamicina	14353503	13
Caelo	Sulfato de gentamicina	14353504	12
Caelo	Sulfato de gentamicina	14353505	3
Caelo	Sulfato de gentamicina	14E08-B03-294841	1
Caelo	Sulfato de gentamicina	14K28-B06-303636	1
Caelo	Sulfato de gentamicina	14K28-B06-303646	3
Caelo	Sulfato de gentamicina	150320G	1
Caelo	Sulfato de gentamicina	1506016-01	2
Caelo	Sulfato de gentamicina	1506016-02	2
Caelo	Sulfato de gentamicina	15128818	1
Caelo	Sulfato de gentamicina	15226501	20
Caelo	Sulfato de gentamicina	15226502	15
Caelo	Sulfato de gentamicina	1522650217099604	1
Caelo	Sulfato de gentamicina	15226508	2
Caelo	Sulfato de gentamicina	15226513	1
Caelo	Sulfato de gentamicina	15226514	5
Caelo	Sulfato de gentamicina	15226517	1
Caelo	Sulfato de gentamicina	15226518	9
Caelo	Sulfato de gentamicina	15258802	15
Caelo	Sulfato de gentamicina	15258803	17
Caelo	Sulfato de gentamicina	15258805	2
Caelo	Sulfato de gentamicina	15258808	10
Caelo	Sulfato de gentamicina	15258809	1
Caelo	Sulfato de gentamicina	15258810	18
Caelo	Sulfato de gentamicina	15258813	14
Caelo	Sulfato de gentamicina	15258815	3
Caelo	Sulfato de gentamicina	15258816	16
Caelo	Sulfato de gentamicina	15258818	33
Caelo	Sulfato de gentamicina	15258819	6
Caelo	Sulfato de gentamicina	15258825	2
Caelo	Sulfato de gentamicina	1528802	1
Caelo	Sulfato de gentamicina	1528818	1
Caelo	Sulfato de gentamicina	15B03-B07-309482	1
Caelo	Sulfato de gentamicina	1604054-01	3
Caelo	Sulfato de gentamicina	1604054-02	1
Caelo	Sulfato de gentamicina	1604054-03	1
Caelo	Sulfato de gentamicina	1610036-01	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de gentamicina	161003602	1
Caelo	Sulfato de gentamicina	16119302	1
Caelo	Sulfato de gentamicina	16b29-b01-328731	1
Caelo	Sulfato de gentamicina	16B29-B01-328731	1
Caelo	Sulfato de gentamicina	17081502	1
Caelo	Sulfato de gentamicina	1709601	1
Caelo	Sulfato de gentamicina	17099601	3
Caelo	Sulfato de gentamicina	17099603	28
Caelo	Sulfato de gentamicina	17099604	19
Caelo	Sulfato de gentamicina	17099606	20
Caelo	Sulfato de gentamicina	17099606-20180404Ma1	1
Caelo	Sulfato de gentamicina	17099608	24
Caelo	Sulfato de gentamicina	1710I-01582	1
Caelo	Sulfato de gentamicina	1711025	1
Caelo	Sulfato de gentamicina	1711025-01	2
Caelo	Sulfato de gentamicina	1711025-02	4
Caelo	Sulfato de gentamicina	17332419	1
Caelo	Sulfato de gentamicina	17358603	35
Caelo	Sulfato de gentamicina	17358604	12
Caelo	Sulfato de gentamicina	17358607	2
Caelo	Sulfato de gentamicina	17358609	39
Caelo	Sulfato de gentamicina	17358609P-180201-2	1
Caelo	Sulfato de gentamicina	17358610	11
Caelo	Sulfato de gentamicina	17358616	37
Caelo	Sulfato de gentamicina	17358618	14
Caelo	Sulfato de gentamicina	17358619	1
Caelo	Sulfato de gentamicina	17358623	1
Caelo	Sulfato de gentamicina	17358909	1
Caelo	Sulfato de gentamicina	1800104	1
Caelo	Sulfato de gentamicina	18041804	1
Caelo	Sulfato de gentamicina	180801301	2
Caelo	Sulfato de gentamicina	1808013-01	2
Caelo	Sulfato de gentamicina	183001001	1
Caelo	Sulfato de gentamicina	183001002	1
Caelo	Sulfato de gentamicina	183001004	20
Caelo	Sulfato de gentamicina	18300103	7
Caelo	Sulfato de gentamicina	18300104	26
Caelo	Sulfato de gentamicina	18300108	12
Caelo	Sulfato de gentamicina	18300109	40
Caelo	Sulfato de gentamicina	183001112	1
Caelo	Sulfato de gentamicina	18300112	28
Caelo	Sulfato de gentamicina	18300113	27
Caelo	Sulfato de gentamicina	18300114	9
Caelo	Sulfato de gentamicina	18399104	1
Caelo	Sulfato de gentamicina	18C12-B02-349026	1
Caelo	Sulfato de gentamicina	18G06-B09-354797	1
Caelo	Sulfato de gentamicina	18Go6-351916	1
Caelo	Sulfato de gentamicina	190703601	1
Caelo	Sulfato de gentamicina	1907036-01	1
Caelo	Sulfato de gentamicina	192564002	29
Caelo	Sulfato de gentamicina	192564003	19
Caelo	Sulfato de gentamicina	192564004	2
Caelo	Sulfato de gentamicina	192564008	1
Caelo	Sulfato de gentamicina	192564009	7
Caelo	Sulfato de gentamicina	192564010	21
Caelo	Sulfato de gentamicina	19256402	1
Caelo	Sulfato de gentamicina	19300109	1
Caelo	Sulfato de gentamicina	19300113	1
Caelo	Sulfato de gentamicina	200004483010	1
Caelo	Sulfato de gentamicina	20004482002	21

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de gentamicina	20004482004	6
Caelo	Sulfato de gentamicina	20004483	1
Caelo	Sulfato de gentamicina	20004483001	37
Caelo	Sulfato de gentamicina	200044830014	1
Caelo	Sulfato de gentamicina	20004483005	12
Caelo	Sulfato de gentamicina	20004483006	1
Caelo	Sulfato de gentamicina	20004483007	15
Caelo	Sulfato de gentamicina	20004483008	1
Caelo	Sulfato de gentamicina	20004483009	8
Caelo	Sulfato de gentamicina	20004483010	22
Caelo	Sulfato de gentamicina	20004483011	1
Caelo	Sulfato de gentamicina	20004483012	1
Caelo	Sulfato de gentamicina	20004483013	4
Caelo	Sulfato de gentamicina	20004483014	21
Caelo	Sulfato de gentamicina	2000448310	1
Caelo	Sulfato de gentamicina	2003058-02	1
Caelo	Sulfato de gentamicina	2004483009	1
Caelo	Sulfato de gentamicina	2004483014	2
Caelo	Sulfato de gentamicina	20161102-4	1
Caelo	Sulfato de gentamicina	20170829/1	1
Caelo	Sulfato de gentamicina	2200075400	1
Caelo	Sulfato de gentamicina	22000754001	16
Caelo	Sulfato de gentamicina	22000754003	11
Caelo	Sulfato de gentamicina	22000754006	11
Caelo	Sulfato de gentamicina	22000754012	1
Caelo	Sulfato de gentamicina	2200754001	1
Caelo	Sulfato de gentamicina	23012015E	1
Caelo	Sulfato de gentamicina	2794	1
Caelo	Sulfato de gentamicina	31032014E	1
Caelo	Sulfato de gentamicina	3110806	1
Caelo	Sulfato de gentamicina	312012	1
Caelo	Sulfato de gentamicina	3265	1
Caelo	Sulfato de gentamicina	3714I-01582	1
Caelo	Sulfato de gentamicina	4563125	1
Caelo	Sulfato de gentamicina	6082013C	1
Caelo	Sulfato de gentamicina	7011505	1
Caelo	Sulfato de gentamicina	73402189	1
Caelo	Sulfato de gentamicina	8702	1
Caelo	Sulfato de gentamicina	B18-1955204	1
Caelo	Sulfato de gentamicina	FG1503073	1
Caelo	Sulfato de gentamicina	FG1603072	1
Caeol/ Noweda	Sulfato de gentamicina	15258803	2
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300113	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564010	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	17358603	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	183001004	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	17358609	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483005	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300109	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004482002	1
Caesar & Loretz GmbH/AEP	Sulfato de gentamicina	20004483010	1
Caesar & Loretz GmbH/Gehe	Sulfato de gentamicina	20004483014	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483010	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004482004	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483009	1
Caesar & Loretz GmbH/Kehr	Sulfato de gentamicina	18300112	1
Caesar & Loretz GmbH/Kehr	Sulfato de gentamicina	192564010	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564010	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300104	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300113	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300104	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300114	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564002	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564008	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483005	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483013	1
Caesar & Loretz GmbH/Otto	Sulfato de gentamicina	192564003	1
Caesar & Loretz GmbH/Ph	Sulfato de gentamicina	183001004	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564010	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300112	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300113	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483001	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483007	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	22000754003	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	18300108	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564002	2
Caesar & Loretz GmbH...	Sulfato de gentamicina	183001004	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	192564010	2
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004482002	3
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483001	3
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483005	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483010	1
Caesar & Loretz GmbH...	Sulfato de gentamicina	20004483014	1
Caesar & Loretz GmbH	Sulfato de gentamicina	14353503	1
Caesar & Loretz GmbH	Sulfato de gentamicina	17099604	1
Caesar & Loretz GmbH	Sulfato de gentamicina	17358607	1
Caesar & Loretz GmbH	Sulfato de gentamicina	17358609	1
Caesar & Loretz GmbH	Sulfato de gentamicina	17358610	1
Caesar & Loretz GmbH	Sulfato de gentamicina	17358616	5
Caesar & Loretz GmbH	Sulfato de gentamicina	17358618	3
Caesar & Loretz GmbH	Sulfato de gentamicina	17358619	1
Caesar & Loretz GmbH	Sulfato de gentamicina	183001002	4
Caesar & Loretz GmbH	Sulfato de gentamicina	183001004	14
Caesar & Loretz GmbH	Sulfato de gentamicina	18300103	1
Caesar & Loretz GmbH	Sulfato de gentamicina	18300104	11
Caesar & Loretz GmbH	Sulfato de gentamicina	18300108	3
Caesar & Loretz GmbH	Sulfato de gentamicina	18300109	6
Caesar & Loretz GmbH	Sulfato de gentamicina	18300110	2
Caesar & Loretz GmbH	Sulfato de gentamicina	18300112	10
Caesar & Loretz GmbH	Sulfato de gentamicina	18300113	7
Caesar & Loretz GmbH	Sulfato de gentamicina	18300114	5
Caesar & Loretz GmbH	Sulfato de gentamicina	192564002	8
Caesar & Loretz GmbH	Sulfato de gentamicina	192564003	3
Caesar & Loretz GmbH	Sulfato de gentamicina	192564006	1
Caesar & Loretz GmbH	Sulfato de gentamicina	192564008	2
Caesar & Loretz GmbH	Sulfato de gentamicina	192564009	4
Caesar & Loretz GmbH	Sulfato de gentamicina	192564010	10
Caesar & Loretz GmbH	Sulfato de gentamicina	19256410	1
Caesar & Loretz GmbH	Sulfato de gentamicina	20004482002	6
Caesar & Loretz GmbH	Sulfato de gentamicina	20004482004	5
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483001	11
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483002	1
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483005	3
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483007	4
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483009	5
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483010	13
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483012	3
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483013	7
Caesar & Loretz GmbH	Sulfato de gentamicina	20004483014	6
Caesar & Loretz GmbH	Sulfato de gentamicina	20004486010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sulfato de gentamicina	22000754001	3
Caesar & Loretz GmbH	Sulfato de gentamicina	22000754003	7
Caesar & Loretz GmbH	Sulfato de gentamicina	22000754006	6
Caesar & Loretz	Sulfato de gentamicina	17358603	1
Caesar & Loretz	Sulfato de gentamicina	20004483007	1
Caesar / Ebert	Sulfato de gentamicina	15258818	1
Caesar&Loretz GmbH,2...	Sulfato de gentamicina	15258802	1
Caesar&Loretz GmbH	Sulfato de gentamicina	15226501	1
Caesar&Loretz GmbH	Sulfato de gentamicina	1907036-01	1
Caleo/ Noweda	Sulfato de gentamicina	17099606	1
Cealo / Anzag	Sulfato de gentamicina	211108(20004483007)	1
Cealo	Sulfato de gentamicina		1
Celo/Jenne	Sulfato de gentamicina	17099603	1
CL/Gehe	Sulfato de gentamicina	17358616	1
Delta Apotheke	Sulfato de gentamicina	17358604	2
Ebert & Jacobi	Sulfato de gentamicina	1506016-01	1
EuRho / Gehe	Sulfato de gentamicina	2003058-02	2
EuRho / Phönix	Sulfato de gentamicina	1610036-02	1
Eurho AHD 20.11.19 E...	Sulfato de gentamicina	1808013-02	1
Eurho Phönix	Sulfato de gentamicina	2107013-2	1
EuRho/Gehe	Sulfato de gentamicina	2003058-01	1
EuRho/Gehe	Sulfato de gentamicina	2003058-02	2
EuRho/Krieger	Sulfato de gentamicina	1711025-02	1
Eurho/Noweda	Sulfato de gentamicina	1604054-02	1
EuRho/Noweda	Sulfato de gentamicina	1907036-01	2
EuRho/Phoenix	Sulfato de gentamicina	1808013-02	1
Eurho/Phönix	Sulfato de gentamicina	200305802	1
EuRho/Phönix	Sulfato de gentamicina	2003058-02	1
EuRho	Sulfato de gentamicina	1106016-03	1
EuRho	Sulfato de gentamicina	1305047-01	1
eurho	Sulfato de gentamicina	1711025-01	1
EuRho	Sulfato de gentamicina	1711025-01	2
EuRho	Sulfato de gentamicina	1808013-01	4
EuRho	Sulfato de gentamicina	190703601	1
EuRho	Sulfato de gentamicina	1907036-01	2
EuRho	Sulfato de gentamicina	2203032-01	1
EuRho	Sulfato de gentamicina	FG1112482	1
Eurimpharm1	Sulfato de gentamicina	1604054-01	1
euro AHD	Sulfato de gentamicina	1711025-015586	1
Euro Gehe	Sulfato de gentamicina	1907036-01	1
Euro Noweda	Sulfato de gentamicina	FG1802035	1
Euro OTC	Sulfato de gentamicina		1
Euro OTC	Sulfato de gentamicina	1106016-01	3
Euro OTC	Sulfato de gentamicina	1106016-02	3
Euro OTC	Sulfato de gentamicina	1106016-03	5
Euro OTC	Sulfato de gentamicina	1205021-01	12
Euro OTC	Sulfato de gentamicina	1205021-02	17
Euro OTC	Sulfato de gentamicina	1305047	1
Euro OTC	Sulfato de gentamicina	130504701	1
Euro OTC	Sulfato de gentamicina	1305047-01	9
Euro OTC	Sulfato de gentamicina	130504703	2
Euro OTC	Sulfato de gentamicina	1305047-03	12
Euro OTC	Sulfato de gentamicina	13189607	1
Euro OTC	Sulfato de gentamicina	1407024	1
Euro OTC	Sulfato de gentamicina	1407024-01	6
Euro OTC	Sulfato de gentamicina	1407024-02	1
Euro OTC	Sulfato de gentamicina	140702403	1
Euro OTC	Sulfato de gentamicina	1407024-03	2
Euro OTC	Sulfato de gentamicina	140702404	3
Euro OTC	Sulfato de gentamicina	1407024-04	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sulfato de gentamicina	150601601	1
Euro OTC	Sulfato de gentamicina	1506016-01	18
Euro OTC	Sulfato de gentamicina	150601602	2
Euro OTC	Sulfato de gentamicina	1506016-02	29
Euro OTC	Sulfato de gentamicina	15258816	2
Euro OTC	Sulfato de gentamicina	160405-03	1
Euro OTC	Sulfato de gentamicina	160405401	1
Euro OTC	Sulfato de gentamicina	1604054-01	25
Euro OTC	Sulfato de gentamicina	1604054-02	13
Euro OTC	Sulfato de gentamicina	1604054-03	3
Euro OTC	Sulfato de gentamicina	1604054-3	1
Euro OTC	Sulfato de gentamicina	161003601	3
Euro OTC	Sulfato de gentamicina	1610036-01	22
Euro OTC	Sulfato de gentamicina	1610036-015339	1
Euro OTC	Sulfato de gentamicina	161003602	1
Euro OTC	Sulfato de gentamicina	1610036-02	17
Euro OTC	Sulfato de gentamicina	171025-02	1
Euro OTC	Sulfato de gentamicina	1711025-01	37
Euro OTC	Sulfato de gentamicina	171102502	1
Euro OTC	Sulfato de gentamicina	1711025-02	16
Euro OTC	Sulfato de gentamicina	17358609	2
Euro OTC	Sulfato de gentamicina	1801813-02	1
Euro OTC	Sulfato de gentamicina	180208G/1711025-01	1
Euro OTC	Sulfato de gentamicina	1808013-01	27
Euro OTC	Sulfato de gentamicina	180801302	2
Euro OTC	Sulfato de gentamicina	1808013-02	35
Euro OTC	Sulfato de gentamicina	180813-02	1
Euro OTC	Sulfato de gentamicina	18C12-B02-349519	1
Euro OTC	Sulfato de gentamicina	18G06-B09	1
Euro OTC	Sulfato de gentamicina	1907035-01	1
Euro OTC	Sulfato de gentamicina	1907036	2
Euro OTC	Sulfato de gentamicina	190703601	6
Euro OTC	Sulfato de gentamicina	1907036-01	54
Euro OTC	Sulfato de gentamicina	1907038-01	1
Euro OTC	Sulfato de gentamicina	20003058-01	1
Euro OTC	Sulfato de gentamicina	2003052-01	1
Euro OTC	Sulfato de gentamicina	2003053-01	1
Euro OTC	Sulfato de gentamicina	2003058	3
Euro OTC	Sulfato de gentamicina	2003058-01	46
Euro OTC	Sulfato de gentamicina	200305802	2
Euro OTC	Sulfato de gentamicina	2003058-02	58
Euro OTC	Sulfato de gentamicina	2003058-42	1
Euro OTC	Sulfato de gentamicina	2107013-01	7
Euro OTC	Sulfato de gentamicina	2107013-02	18
Euro OTC	Sulfato de gentamicina	22000754003	1
Euro OTC	Sulfato de gentamicina	2203032-01	6
Euro OTC	Sulfato de gentamicina	2911034-02	1
Euro OTC	Sulfato de gentamicina	4318A-01582	1
Euro OTC	Sulfato de gentamicina	4988304	1
Euro OTC	Sulfato de gentamicina	80616-2	1
Euro OTC	Sulfato de gentamicina	FG11112482	1
Euro OTC	Sulfato de gentamicina	FG1501009	1
Euro OTC	Sulfato de gentamicina	FG1706157	1
Euro OTC	Sulfato de gentamicina	FG1709241	2
Euro OTC	Sulfato de gentamicina	FG1802035	1
Euro/Krieger	Sulfato de gentamicina	1711025-02	1
Euro/Phönix	Sulfato de gentamicina	1808013-01	1
Euro/Phönix	Sulfato de gentamicina	1907036-01	1
Euro/Phönix	Sulfato de gentamicina	2003058-0208	1
Euro/Sana	Sulfato de gentamicina	1808013-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRoh/ Gehe	Sulfato de gentamicina	17358616	1
EuRoh/ Gehe	Sulfato de gentamicina	190703601	1
Euroo/Noweda	Sulfato de gentamicina	2003058-02	1
Euroo/Phoenix	Sulfato de gentamicina	1305047-03	1
Fagron	Sulfato de gentamicina		1
Fagron	Sulfato de gentamicina	10A29-N06	1
Fagron	Sulfato de gentamicina	10C22N02	1
Fagron	Sulfato de gentamicina	11/09-N10	1
Fagron	Sulfato de gentamicina	1106016-01	1
Fagron	Sulfato de gentamicina	11604054-01	1
Fagron	Sulfato de gentamicina	11k21-n17	1
Fagron	Sulfato de gentamicina	11K21-N17	2
Fagron	Sulfato de gentamicina	1205021-02	1
Fagron	Sulfato de gentamicina	1221-n02	1
Fagron	Sulfato de gentamicina	12B21-N02	2
Fagron	Sulfato de gentamicina	12D26-N05	9
Fagron	Sulfato de gentamicina	12D6-N05	1
Fagron	Sulfato de gentamicina	12G04-N16	2
Fagron	Sulfato de gentamicina	12117-no2	1
Fagron	Sulfato de gentamicina	13/19-B05	1
Fagron	Sulfato de gentamicina	13/19-B05-286568	1
Fagron	Sulfato de gentamicina	13189607	1
Fagron	Sulfato de gentamicina	1319-B05-286565	1
Fagron	Sulfato de gentamicina	13D24-N05	8
Fagron	Sulfato de gentamicina	13F13-N01	1
Fagron	Sulfato de gentamicina	13I19-B05	1
Fagron	Sulfato de gentamicina	13I19-B05-286568	1
Fagron	Sulfato de gentamicina	14081307	2
Fagron	Sulfato de gentamicina	14A30-B04	3
Fagron	Sulfato de gentamicina	14a30-b04-290858	1
Fagron	Sulfato de gentamicina	14A30-B04-290858	1
Fagron	Sulfato de gentamicina	14A30-B04-290861	2
Fagron	Sulfato de gentamicina	14E08-B03	2
Fagron	Sulfato de gentamicina	14E08-B03-294835	2
Fagron	Sulfato de gentamicina	14E08-B03-294841	1
Fagron	Sulfato de gentamicina	14E08-B03-294848	5
Fagron	Sulfato de gentamicina	14e08b03300619	1
Fagron	Sulfato de gentamicina	14E08-B03-300619	1
Fagron	Sulfato de gentamicina	14K28-B06	3
Fagron	Sulfato de gentamicina	14K28-B06_303646	1
Fagron	Sulfato de gentamicina	14K28-B06-301951	1
Fagron	Sulfato de gentamicina	14k28-b06-303640	2
Fagron	Sulfato de gentamicina	14k28-B06-303640	1
Fagron	Sulfato de gentamicina	14K28-B06-303640	4
Fagron	Sulfato de gentamicina	14K28B06303646	2
Fagron	Sulfato de gentamicina	14K28-B06-303646	5
Fagron	Sulfato de gentamicina	15121722	2
Fagron	Sulfato de gentamicina	15258802	1
Fagron	Sulfato de gentamicina	15258816	2
Fagron	Sulfato de gentamicina	15803-B07-309482	1
Fagron	Sulfato de gentamicina	15B03-B07	1
Fagron	Sulfato de gentamicina	15b03-b07-309482	1
Fagron	Sulfato de gentamicina	15B03-B07-309482	2
Fagron	Sulfato de gentamicina	15E04-B05-316255	2
Fagron	Sulfato de gentamicina	15E04-B05-319740	1
Fagron	Sulfato de gentamicina	15G29-B09-320305	3
Fagron	Sulfato de gentamicina	15G29-B09-322928	1
Fagron	Sulfato de gentamicina	15G29B09322936	1
Fagron	Sulfato de gentamicina	15G29-B09-322936	2
Fagron	Sulfato de gentamicina	15G29-B09-322945	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de gentamicina	15G29B0932632	1
Fagron	Sulfato de gentamicina	15G29-B09-326632	4
Fagron	Sulfato de gentamicina	15G29-B09-326635	2
Fagron	Sulfato de gentamicina	16829-B01-328731	1
Fagron	Sulfato de gentamicina	16B29-B01	1
Fagron	Sulfato de gentamicina	16B29-B01-328731	4
Fagron	Sulfato de gentamicina	16-B-29-B01-328731	1
Fagron	Sulfato de gentamicina	16b29-b01-328915	1
Fagron	Sulfato de gentamicina	16B29-B01-328915	2
Fagron	Sulfato de gentamicina	17099606	1
Fagron	Sulfato de gentamicina	17099608	1
Fagron	Sulfato de gentamicina	1711025-01	1
Fagron	Sulfato de gentamicina	17G27-B05	1
Fagron	Sulfato de gentamicina	17G27-B05-340121	2
Fagron	Sulfato de gentamicina	17k16-B09-343323	1
Fagron	Sulfato de gentamicina	17K16-B09-343323	1
Fagron	Sulfato de gentamicina	17K-16-B09-343323	1
Fagron	Sulfato de gentamicina	180810051	1
Fagron	Sulfato de gentamicina	18C12-B02	3
Fagron	Sulfato de gentamicina	18C12-B02-349025	7
Fagron	Sulfato de gentamicina	18C12-B02-349026	2
Fagron	Sulfato de gentamicina	18C12-B02-349519	1
Fagron	Sulfato de gentamicina	18C12-B02-350	1
Fagron	Sulfato de gentamicina	18C12B02350204	1
Fagron	Sulfato de gentamicina	18C12-B02-350204	4
Fagron	Sulfato de gentamicina	18G06-B09	2
Fagron	Sulfato de gentamicina	18G06-B09-351916	6
Fagron	Sulfato de gentamicina	18G06-B09-354797	9
Fagron	Sulfato de gentamicina	1914Q-01582	1
Fagron	Sulfato de gentamicina	19A22-B05-191434	18
Fagron	Sulfato de gentamicina	19-B05-286568	1
Fagron	Sulfato de gentamicina	19G17-805-193462	1
Fagron	Sulfato de gentamicina	19G17-B05-193462	7
Fagron	Sulfato de gentamicina	19G17-BO5-193462	2
Fagron	Sulfato de gentamicina	19J15-B18-195524	2
Fagron	Sulfato de gentamicina	2003058-02	1
Fagron	Sulfato de gentamicina	20820-801-197708	1
Fagron	Sulfato de gentamicina	20B20-B01	1
Fagron	Sulfato de gentamicina	20B20-B01-1977008	1
Fagron	Sulfato de gentamicina	20B20-B01-197708	12
Fagron	Sulfato de gentamicina	20B20-B01-200399	1
Fagron	Sulfato de gentamicina	20B20-B1-197708	1
Fagron	Sulfato de gentamicina	20G27-802-202130	1
Fagron	Sulfato de gentamicina	20G27-B02-201922	3
Fagron	Sulfato de gentamicina	20G27-B02-202130	1
Fagron	Sulfato de gentamicina	2107013-02	1
Fagron	Sulfato de gentamicina	210920013	1
Fagron	Sulfato de gentamicina	21D23-B07-213630	3
Fagron	Sulfato de gentamicina	21D23-B07-215441	1
Fagron	Sulfato de gentamicina	21I20-B09	1
Fagron	Sulfato de gentamicina	21I20-B09-213601	2
Fagron	Sulfato de gentamicina	22C17-B10-218675	2
Fagron	Sulfato de gentamicina	22C17-B10-223074	1
Fagron	Sulfato de gentamicina	22F28-B02-223061	2
Fagron	Sulfato de gentamicina	5214A-01582	1
Fagron	Sulfato de gentamicina	B01-1977008	2
Fagron	Sulfato de gentamicina	B02-2019202	2
Fagron	Sulfato de gentamicina	B02-3502004	2
Fagron	Sulfato de gentamicina	B05-1934602	3
Fagron	Sulfato de gentamicina	B09-3547907	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de gentamicina	FG1212646	1
Fagron	Sulfato de gentamicina	FG1305122	1
Fagron	Sulfato de gentamicina	FG1709255	1
Fagron	Sulfato de gentamicina	FG1711309	2
Fargon	Sulfato de gentamicina	13D24-N05	1
Fargon	Sulfato de gentamicina	16b29-b01-328915	1
Fargon	Sulfato de gentamicina	190110014	1
Fargron/AHD	Sulfato de gentamicina	12G04-N16	1
Fuijan/Noweda	Sulfato de gentamicina	18300108	1
Fuijan/Noweda	Sulfato de gentamicina	192564009	1
Fuijan/Noweda	Sulfato de gentamicina	FG1709243	3
Fujan	Sulfato de gentamicina	2003058-02	1
Fujian FP / Gehe	Sulfato de gentamicina	192564002	1
Fujian Fukang Pharm....	Sulfato de gentamicina	17358603	1
Fujian Fukang Pharma...	Sulfato de gentamicina	14A30-B04-290861	1
Fujian Fukang Pharma...	Sulfato de gentamicina	14E08-B03-300619	1
Fujian Fukang Pharma...	Sulfato de gentamicina	2003058-02	3
Fujian Fukang Pharma...	Sulfato de gentamicina	12G04-N16	2
Fujian Fukang Pharma...	Sulfato de gentamicina	14E08-B03-294848	1
Fujian/Noweda	Sulfato de gentamicina	FG1802035	2
Fujian	Sulfato de gentamicina	FG1706157	1
Gehe am 24.2.14	Sulfato de gentamicina	1305047-01	1
Gehe amax	Sulfato de gentamicina	1711025-01	1
Gehe amax	Sulfato de gentamicina	2003058-01	1
Gehe/EuRho	Sulfato de gentamicina	2203032-01	1
Gehe/Euro	Sulfato de gentamicina	1610036-02	1
Gehe	Sulfato de gentamicina		1
Gehe	Sulfato de gentamicina	12146604	1
Gehe	Sulfato de gentamicina	13205007	1
Gehe	Sulfato de gentamicina	14353505	1
Gehe	Sulfato de gentamicina	15226517	1
GEHE	Sulfato de gentamicina	15258808	1
GEHE	Sulfato de gentamicina	15258815	1
Gehe	Sulfato de gentamicina	15258818	1
Gehe	Sulfato de gentamicina	15E04-B05-319740	1
Gehe	Sulfato de gentamicina	1610036-01	1
Gehe	Sulfato de gentamicina	17099606	1
Gehe	Sulfato de gentamicina	1711025-01	1
GEHE	Sulfato de gentamicina	17358603	2
Gehe	Sulfato de gentamicina	17358609	1
GEHE	Sulfato de gentamicina	17358609	1
Gehe	Sulfato de gentamicina	1808013-01	1
Gehe	Sulfato de gentamicina	1808013-02	1
Gehe	Sulfato de gentamicina	18300103	1
Gehe	Sulfato de gentamicina	18300108	1
Gehe	Sulfato de gentamicina	18300109	2
GEHE	Sulfato de gentamicina	18300109	1
Gehe	Sulfato de gentamicina	1907036-01	1
Gehe	Sulfato de gentamicina	19A22-B05-191434	1
Gehe	Sulfato de gentamicina	19G17-B05-193462	1
Gehe	Sulfato de gentamicina	20004482004	1
Gehe	Sulfato de gentamicina	2002058-01	1
Gehe	Sulfato de gentamicina	22000754013	2
Gehe	Sulfato de gentamicina	22C17-B10-223074	1
Gehe	Sulfato de gentamicina	FG1307194	1
Geilenkirchen	Sulfato de gentamicina	15258816	1
Geilenkirchen	Sulfato de gentamicina	18300104	1
Hedinger	Sulfato de gentamicina	1711025-01	1
Ichthyol/ALH	Sulfato de gentamicina	15258810	1
Jenne	Sulfato de gentamicina	20004482002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Sulfato de gentamicina	20004483014	1
Jenne	Sulfato de gentamicina	22000754013	1
Jenne	Sulfato de gentamicina	23001024004	1
Kehr	Sulfato de gentamicina	110036-02	1
Kehr	Sulfato de gentamicina	22000754003	1
Klosterring	Sulfato de gentamicina	15G29-B09	1
Mömerzheim	Sulfato de gentamicina	1711025-01	1
Nachprüfung	Sulfato de gentamicina	123456	1
Noweda Taucha	Sulfato de gentamicina	20004483014	1
Noweda Taucha	Sulfato de gentamicina	2003058-02	1
Noweda/ Caesar&Loren…	Sulfato de gentamicina	192564002	1
Noweda	Sulfato de gentamicina	12146602	1
Noweda	Sulfato de gentamicina	1305005	1
Noweda	Sulfato de gentamicina	13189607	1
Noweda	Sulfato de gentamicina	13189611	1
Noweda	Sulfato de gentamicina	13189612	1
Noweda	Sulfato de gentamicina	140702404	1
Noweda	Sulfato de gentamicina	14353504	1
Noweda	Sulfato de gentamicina	15226514	1
Noweda	Sulfato de gentamicina	15258818	1
Noweda	Sulfato de gentamicina	1711025-02	1
Noweda	Sulfato de gentamicina	17358616	2
Noweda	Sulfato de gentamicina	17358623	1
Noweda	Sulfato de gentamicina	18300108	2
Noweda	Sulfato de gentamicina	1907036-01	2
noweda	Sulfato de gentamicina	192564003	1
Noweda	Sulfato de gentamicina	192564003	1
Noweda	Sulfato de gentamicina	20004483013	1
Noweda	Sulfato de gentamicina	210920013	1
Noweda	Sulfato de gentamicina	22000754003	1
Noweda	Sulfato de gentamicina	22000754006	1
Noweda	Sulfato de gentamicina	23001024004	1
ph euro	Sulfato de gentamicina	2003058-01	1
PHOENIX 10.03.2014	Sulfato de gentamicina	1305047	1
Phoenix	Sulfato de gentamicina	12D26-N05	1
Phoenix	Sulfato de gentamicina	1305047-03	1
Phoenix	Sulfato de gentamicina	15226501	1
Phoenix	Sulfato de gentamicina	15226502	1
Phoenix	Sulfato de gentamicina	15258816	1
Phoenix	Sulfato de gentamicina	1604054-02	1
Phoenix	Sulfato de gentamicina	16b29-b01-328731	1
Phoenix	Sulfato de gentamicina	17099603	1
Phoenix	Sulfato de gentamicina	1711025-02	2
phoenix	Sulfato de gentamicina	17358603	1
Phoenix	Sulfato de gentamicina	17358603	1
Phoenix	Sulfato de gentamicina	17G27-B05-340121	1
Phoenix	Sulfato de gentamicina	18300108	1
Phoenix	Sulfato de gentamicina	18300113	1
Phoenix	Sulfato de gentamicina	20004483001	1
Phoenix	Sulfato de gentamicina	2003058-01	1
Phoenix	Sulfato de gentamicina	22000754003	1
Phoenix	Sulfato de gentamicina	23001024005	1
Phoenix	Sulfato de gentamicina	3404	1
Phönix Gotha	Sulfato de gentamicina	13189611	1
Phönix	Sulfato de gentamicina	11113309	1
phönix	Sulfato de gentamicina	1214605	1
Phönix	Sulfato de gentamicina	12146602	1
Phönix	Sulfato de gentamicina	13189611	1
Phönix	Sulfato de gentamicina	14353502	1
PHÖNIX	Sulfato de gentamicina	15226514	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Sulfato de gentamicina	15258818	1
Phönix	Sulfato de gentamicina	17099603	1
Phönix	Sulfato de gentamicina	17099604	1
phönix	Sulfato de gentamicina	18300103	1
Phönix	Sulfato de gentamicina	18300109	2
Phönix	Sulfato de gentamicina	192564009	1
PHÖNIX	Sulfato de gentamicina	20004483001	1
Phönix	Sulfato de gentamicina	2003058-01	2
phönix	Sulfato de gentamicina	22000754006	1
Phönix	Sulfato de gentamicina	22000754013	1
Phönix	Sulfato de gentamicina	23001024004	2
Phönix	Sulfato de gentamicina	3141	1
Sanacorp 06.01.15 EK 6,20	Sulfato de gentamicina	1305047-03	1
Sanacorp WE: 28.09.1…	Sulfato de gentamicina	15258825	1
Sanacorp	Sulfato de gentamicina	1305047-03	1
Sanacorp	Sulfato de gentamicina	13189607	1
Sanacorp	Sulfato de gentamicina	13189608	1
Sanacorp	Sulfato de gentamicina	161003601	1
Sanacorp	Sulfato de gentamicina	1610036-01	2
Sanacorp	Sulfato de gentamicina	1610036-02	1
Sanacorp	Sulfato de gentamicina	161036-02	1
Sanacorp	Sulfato de gentamicina	1711025-02	1
Sanacorp	Sulfato de gentamicina	17358603	1
Sanacorp	Sulfato de gentamicina	17358604	1
Sanacorp	Sulfato de gentamicina	17358618	1
Sanacorp	Sulfato de gentamicina	18300109	1
Sanacorp	Sulfato de gentamicina	18300112	1
sanacorp	Sulfato de gentamicina	18300113	1
Sanacorp	Sulfato de gentamicina	18300113	1
Sanacorp	Sulfato de gentamicina	18C12-B02-349026	1
Sanacorp	Sulfato de gentamicina	19G17-B05-193462	1
Sanacorp	Sulfato de gentamicina	2003058-02	1
Sanacorp	Sulfato de gentamicina	2203032-01	1
Sanacorp	Sulfato de gentamicina	23001024004	1
Sanacorp	Sulfato de gentamicina	23001024005	1
Sanacorp	Sulfato de gentamicina	FG1711309	1
vdl	Sulfato de gentamicina	12146602	1
Yantai Justaware Ph.…	Sulfato de gentamicina	14081307	1
Yantai Justaware Ph.…	Sulfato de gentamicina	14K28-B06_303646	1
Yantai Justaware Pha…	Sulfato de gentamicina	14K28-B06	1

- 233 530 spectra from 1515 *Apo-Ident* customers from a total of 48 881 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de gentamicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de gentamicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	1015	0	151 947
Type B	0	948	2	201 134
Type C	0	2447	90	233 530

The substance/substance group *Sulfato de gentamicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4089 %)
Type B	100.0000 % (> 99.9912 %)	99.7895 % (> 99.4737 %)
Type C	100.0000 % (> 99.9007 %)	96.4525 % (> 96.3343 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20661	20661	0,00	115,09
21081	21837	4,26	118,02
21578	25201	43,04	84,88
21580	21837	7,14	115,85
21582	21582	0,00	113,69
21684	21582	5,22	113,06
21697	21697	0,00	111,94
21837	21837	0,00	114,16
22604	21837	3,65	117,53
22857	22857	0,00	126,51
23210	21837	6,91	115,20
23782	23782	0,00	116,07
23882	23882	0,00	114,56
24866	24866	0,00	114,11
25180	22857	21,51	122,85
25201	25201	0,00	99,34
25252	25252	0,00	118,07
25638	25638	0,00	96,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de glicosamina cloreto de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006689-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de glicosamina cloreto de potássio; Sulfato de glucosamina cloreto de potássio

Special notes

When selecting the *Sulfato de glicosamina cloreto de potássio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de glicosamina cloreto de potássio	2	1	0

Second-stage model

For differentiation of the substance/substance group *Sulfato de glicosamina cloreto de potássio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de glicosamina cloreto de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	104,19	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de glicosamina cloreto de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de glicosamina cloreto de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulfato de glicosamina cl…	TSM-K-2404002	BR20047	40	20240928*
Fagron	Sulfato de glicosamina cl…	TSM-K-2404001	BR20049	40	20240928*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Sulfato de glicosamina cloreto de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 4 reference samples from the substance/substance group *Sulfato de glicosamina cloreto de potássio*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Sulfato de glicosamina cl…	TSM-K-2404003	BR20048	40
Fagron	Sulfato de glicosamina cl…	TSM-K-2404002	BR20047SI†	20
Fagron	Sulfato de glicosamina cl…	TSM-K-2404003	BR20048SI	20
Fagron	Sulfato de glicosamina cl…	TSM-K-2404001	BR20049SI†	20

- 201 984 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sulfato de glicosamina cloreto de potássio*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de glicosamina cloreto de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de glicosamina cloreto de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	100	0	201 984
Type C	0	0	0	236 067

The substance/substance group *Sulfato de glicosamina cloreto de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
BR20047	BR20047	0,00	318,42
BR20049	BR20049	0,00	312,23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de magnésio hepta-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20165-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de magnésio hepta-hidratado; Magnesii sulfas heptahydricus

Special notes

When selecting the *Sulfato de magnésio hepta-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de magnésio hepta-hidratado	6	2	52

Second-stage model

For differentiation of the substance/substance group *Sulfato de magnésio hepta-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de magnésio hepta-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de zinco hepta-hidratado	34,24	–
Cromoglicato de sódio	50,93	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de magnésio hepta-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de magnésio hepta-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de magnésio hepta…	22000334	26054	40	20220301*
Caelo	Sulfato de magnésio hepta…	21002002	26055	40	20210923*
Caelo	Sulfato de magnésio hepta…	22003020	26561	40	20221207*
Caelo	Sulfato de magnésio hepta…	22003020	26561SI	20	20221207*
Caelo	Sulfato de magnésio hepta…	23003364	27105	40	20240124*
Caelo	Sulfato de magnésio hepta…	24002186	27431	40	20241011*
Euro OTC	Sulfato de magnésio hepta…	2308013	26882	40	20230829*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Sulfato de magnésio hepta-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 110 spectra of 4 reference samples from the substance/substance group *Sulfato de magnésio hepta-hidratado*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de magnésio hepta…	23001612	26849	40
Euro OTC	Sulfato de magnésio hepta…	2107026	25789	50
Caelo	Sulfato de magnésio hepta…	22000334	26054SI†	10
Caelo	Sulfato de magnésio hepta…	21002002	26055SI†	10

- 201 974 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 126 spectra from 65 *Apo-Ident* customers from 52 batches from the substance/substance group *Sulfato de magnésio hepta-hidratado*.

- Among them are spectra of independent samples from 52 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Sulfato de magnésio hepta…	1401029-01	1
	Sulfato de magnésio hepta…	21002002005	1
	Sulfato de magnésio hepta…	22001077002	4
	Sulfato de magnésio hepta…	22003025001	2
	Sulfato de magnésio hepta…	22003025003	10
	Sulfato de magnésio hepta…	2210012-01	2
	Sulfato de magnésio hepta…	3134859	1
Anzag 29.04.13 ek: 4,55EUR	Sulfato de magnésio hepta…	12138518	1
Anzag	Sulfato de magnésio hepta…	204035	1
BfB	Sulfato de magnésio hepta…	12L10-N07	2
Bombastus	Sulfato de magnésio hepta…	277424	1
Caelo	Sulfato de magnésio hepta…	10104201	1
Caelo	Sulfato de magnésio hepta…	10371111	1
Caelo	Sulfato de magnésio hepta…	11194001	1
Caelo	Sulfato de magnésio hepta…	11369252	1
Caelo	Sulfato de magnésio hepta…	11369509	1
Caelo	Sulfato de magnésio hepta…	11369525	6
Caelo	Sulfato de magnésio hepta…	11369526	12
Caelo	Sulfato de magnésio hepta…	11369529	1
Caelo	Sulfato de magnésio hepta…	113695625	1
Caelo	Sulfato de magnésio hepta…	1206019-01	4
Caelo	Sulfato de magnésio hepta…	12119901/2	1
Caelo	Sulfato de magnésio hepta…	12138518	2
Caelo	Sulfato de magnésio hepta…	12138521	2
Caelo	Sulfato de magnésio hepta…	1213E-01835	1
Caelo	Sulfato de magnésio hepta…	12336914	5
Caelo	Sulfato de magnésio hepta…	12336915	3
Caelo	Sulfato de magnésio hepta…	12336926	1
Caelo	Sulfato de magnésio hepta…	12c27-n06	1
Caelo	Sulfato de magnésio hepta…	13030104	1
Caelo	Sulfato de magnésio hepta…	13030107	1
Caelo	Sulfato de magnésio hepta…	13183702	2
Caelo	Sulfato de magnésio hepta…	6012014B	1
Caelo	Sulfato de magnésio hepta…	90744129	1
EuRho/Jenne	Sulfato de magnésio hepta…	1202017-01	1
EuRho	Sulfato de magnésio hepta…	1206019-01	1
EuRho	Sulfato de magnésio hepta…	1303008-01	2
EuRho	Sulfato de magnésio hepta…	3512M-01835	1
Euro / Jenne	Sulfato de magnésio hepta…	1401029-01	1
Euro OTC	Sulfato de magnésio hepta…	1109023-01	1
Euro OTC	Sulfato de magnésio hepta…	1202017-01	5
Euro OTC	Sulfato de magnésio hepta…	1211022-01	3
Euro OTC	Sulfato de magnésio hepta…	130300801	1
Euro OTC	Sulfato de magnésio hepta…	1303008-01	3
Euro OTC	Sulfato de magnésio hepta…	1306015-01	1
Euro OTC	Sulfato de magnésio hepta…	170610	1
Fagron	Sulfato de magnésio hepta…	12E22-N02	3
Fagron	Sulfato de magnésio hepta…	12G24-N02	1
Fagron	Sulfato de magnésio hepta…	12L10-N07	6
Fagron	Sulfato de magnésio hepta…	12L10-NO7	1
Fagron	Sulfato de magnésio hepta…	13H05-N02	1
Fagron	Sulfato de magnésio hepta…	26251	1
Fagron	Sulfato de magnésio hepta…	31161	1
fargon	Sulfato de magnésio hepta…	12E22-N02	1
Gehe	Sulfato de magnésio hepta…	12138521	2
Gehe	Sulfato de magnésio hepta…	21002002001	1
Hedinger	Sulfato de magnésio hepta…	204036	1
Hedinger	Sulfato de magnésio hepta…	204037	2
Noweda / 28.10.13 EuRho	Sulfato de magnésio hepta…	1211022-01	1
Noweda	Sulfato de magnésio hepta…	1109023-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Sulfato de magnésio hepta…	22003025001	1
Phoenix	Sulfato de magnésio hepta…	24000129002	1
Phönix	Sulfato de magnésio hepta…	11369526	1
Phönix	Sulfato de magnésio hepta…	22000333004	1
Sanacorp	Sulfato de magnésio hepta…	22003025001	1

- 235 941 spectra from 1515 *Apo-Ident* customers from a total of 49 207 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de magnésio hepta-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de magnésio hepta-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	110	0	201 974
Type C	0	126	0	235 941

The substance/substance group *Sulfato de magnésio hepta-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.5455 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.2381 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26054	26054	0,00	68,75
26055	26055	0,00	140,36
26561	26561	0,00	66,05
26882	26882	0,00	74,40
27105	27105	0,00	87,07
27431	27431	0,00	77,02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de manganês monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20404-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de manganês monoidratado; Mangani sulfas monohydricus

Special notes

When selecting the *Sulfato de manganês monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de manganês monoidratado	2	1	0

Second-stage model

For differentiation of the substance/substance group *Sulfato de manganês monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de manganês monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	81,92	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de manganês monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de manganês monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de manganês monoi…	171648	24404	40	20170714*
Euro OTC	Sulfato de manganês monoi…	2305003	26771	40	20230630*
Euro OTC	Sulfato de manganês monoi…	2305003	26771SI	20	20230630*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Sulfato de manganês monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 862 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 50 spectra of 2 reference samples from the substance/substance group *Sulfato de manganês monoidratado*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sulfato de manganês monoi…	2202003	26047	40
Euro OTC	Sulfato de manganês monoi…	2202003	26047SI	10

- 202 034 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sulfato de manganês monoidratado*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de manganês monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de manganês*

monoidratado and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	44	6	202 034
Type C	0	0	0	236 067

The substance/substance group *Sulfato de manganês monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	88.0000 % (> 82.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24404	24404	0,00	207,71
26771	26771	0,00	232,83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de neomicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20544-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de neomicina; Neomicina, sulfato; Neomycini sulfas

Special notes

When selecting the *Sulfato de neomicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de neomicina	12	5	223

Second-stage model

For differentiation of the substance/substance group *Sulfato de neomicina* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de neomicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de tobramicina	34,78	29,19
Cromoglicato de sódio	55,07	–
⋮	⋮	⋮
Fosfato de Mg-Ca-K-colamina	>50	59,93
Fosfato sódico de riboflavina hidratado	>50	63,65
Gluconato de zinco	>50	91,37
Sulfato de gentamicina	>50	115,97
Carbômero	>50	116,21
Citrato de magnésio	>50	121,55
Tetraborato de sódio	>50	403,69
Finasterida	>50	1490,52

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de neomicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de neomicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de neomicina	13062923	21814	60	AR-15-FG-016581-01
Caelo	Sulfato de neomicina	13062923	22276	45	20130315
Caelo	Sulfato de neomicina	161650	23856	30	20160629*
Caelo	Sulfato de neomicina	20002248	25643	40	20200923*
Caelo	Sulfato de neomicina	24000508	27222	40	20240416*
Euro OTC	Sulfato de neomicina	1303033-03	21771	60	AR-15-FG-016582-01
Euro OTC	Sulfato de neomicina	1601046	22381	45	20160212*
Fagron	Sulfato de neomicina	14C27-B05-302516	21894	60	1604527
Fagron	Sulfato de neomicina	14C27-B05-302517	21961	60	20140418
Fagron	Sulfato de neomicina	19G23-B03-364716	25185	40	20191007
Fagron	Sulfato de neomicina	22E11-B04-224107	26286	40	20220627

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulfato de neomicina	23C10-B04-219531	26664	40	20230310
Fagron	Sulfato de neomicina	23C10-B04-219531	26664SI	20	20230310
Fagron	Sulfato de neomicina	23G20-B10-233758	27052	40	20230803

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 620 spectra of 14 reference samples from the substance/substance group *Sulfato de neomicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 342 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Sulfato de neomicina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de neomicina	15237602	22389	40
Caelo	Sulfato de neomicina	23000856	26894	40
Euro OTC	Sulfato de neomicina	1802005	23952	40
Euro OTC	Sulfato de neomicina	1903022	24642	40
Euro OTC	Sulfato de neomicina	2003021	25280	40
Caelo	Sulfato de neomicina	23000856	26894SI	20
Fagron	Sulfato de neomicina	22E11-B04-224107	26286SI†	20

- 201 844 spectra from a total of 4039 batches from further 842 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1215 spectra from 539 *Apo-Ident* customers from 239 batches from the substance/substance group *Sulfato de neomicina*.
- Among them are spectra of independent samples from 223 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de neomicina	1303033-03	1
	Sulfato de neomicina	13G09-N07	1
	Sulfato de neomicina	2100321600	1
	Sulfato de neomicina	23000856006	3
	Sulfato de neomicina	23000856007	5
	Sulfato de neomicina	23C10-B04-219532	3
	Sulfato de neomicina	23C10-B04-219532	1
	Sulfato de neomicina	23D14-B03-232374	5
	Sulfato de neomicina	24000508004	1
	Sulfato de neomicina	24000508005	1
	Sulfato de neomicina	B03_2323704	1
	Sulfato de neomicina	GY9146	1
AHD/Euro	Sulfato de neomicina	160104602	1
AHD/Euro	Sulfato de neomicina	1802005	1
AHD	Sulfato de neomicina	11/19-N14	1
AHD	Sulfato de neomicina	14A31-B02-294698	2
AHD	Sulfato de neomicina	1802005-01	2
Alliance Health 13.01.204	Sulfato de neomicina	1303033-01	2
Alliance Healthcare	Sulfato de neomicina	1102043-03	1
Alliance	Sulfato de neomicina	1802005-01	1
Alliance	Sulfato de neomicina	2003021-02	1
ApBetrO/Noweda	Sulfato de neomicina	200302-02	1
apo-ident.;4,45EUR; Sa...	Sulfato de neomicina	1601046-01	1
Ashland/Sanacorp	Sulfato de neomicina	1303033-02	1
aurica/phoenix	Sulfato de neomicina	1102043-02	1
Caelo	Sulfato de neomicina	10157505	5
Caelo	Sulfato de neomicina	10206300	1
Caelo	Sulfato de neomicina	1102043-02	1
Caelo	Sulfato de neomicina	11C21-N10	1
Caelo	Sulfato de neomicina	12175401	4
Caelo	Sulfato de neomicina	12276405	1
Caelo	Sulfato de neomicina	12276410	2
Caelo	Sulfato de neomicina	1303033-02	1
Caelo	Sulfato de neomicina	130303303	3
Caelo	Sulfato de neomicina	1303033-03	3
Caelo	Sulfato de neomicina	13062905	2
Caelo	Sulfato de neomicina	13062908	1
Caelo	Sulfato de neomicina	13062921	1
Caelo	Sulfato de neomicina	13062922	1
Caelo	Sulfato de neomicina	13062923	6
Caelo	Sulfato de neomicina	13D10N05	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de neomicina	13G09-N07	1
Caelo	Sulfato de neomicina	14A31-B02-294696	1
Caelo	Sulfato de neomicina	1502004-01	1
Caelo	Sulfato de neomicina	1502004-03	2
Caelo	Sulfato de neomicina	15237602	7
Caelo	Sulfato de neomicina	15298902	2
Caelo	Sulfato de neomicina	15J09-B04-314015	1
Caelo	Sulfato de neomicina	15J27-B07-321372	1
Caelo	Sulfato de neomicina	1601046	1
Caelo	Sulfato de neomicina	1601046-01	3
Caelo	Sulfato de neomicina	1601046-02	2
Caelo	Sulfato de neomicina	16122601	3
Caelo	Sulfato de neomicina	16122611	2
Caelo	Sulfato de neomicina	16122612	8
Caelo	Sulfato de neomicina	16122617	1
Caelo	Sulfato de neomicina	16122618	1
Caelo	Sulfato de neomicina	16122623	1
Caelo	Sulfato de neomicina	16165004	4
Caelo	Sulfato de neomicina	16165006	3
Caelo	Sulfato de neomicina	16165008	2
Caelo	Sulfato de neomicina	16165014	1
Caelo	Sulfato de neomicina	161650145351	1
Caelo	Sulfato de neomicina	16165015	1
Caelo	Sulfato de neomicina	16165016	15
Caelo	Sulfato de neomicina	16165017	2
Caelo	Sulfato de neomicina	16165018	7
Caelo	Sulfato de neomicina	16B10-B50-328165	3
Caelo	Sulfato de neomicina	18018704	7
Caelo	Sulfato de neomicina	180200501	1
Caelo	Sulfato de neomicina	1802005-01	9
Caelo	Sulfato de neomicina	18161303	14
Caelo	Sulfato de neomicina	18161304	4
Caelo	Sulfato de neomicina	18161305	6
Caelo	Sulfato de neomicina	18161307	17
Caelo	Sulfato de neomicina	18161309	1
Caelo	Sulfato de neomicina	18161310	8
Caelo	Sulfato de neomicina	18A25-B05-346135	1
Caelo	Sulfato de neomicina	18A25-B05-346138	1
Caelo	Sulfato de neomicina	18G28B05352957	1
Caelo	Sulfato de neomicina	18G28B05354472	1
Caelo	Sulfato de neomicina	191849001	6
Caelo	Sulfato de neomicina	191849003	8
Caelo	Sulfato de neomicina	19184903	18
Caelo	Sulfato de neomicina	20000391004	6
Caelo	Sulfato de neomicina	200003914004	1
Caelo	Sulfato de neomicina	20004305001	11
Caelo	Sulfato de neomicina	20004305005	9
Caelo	Sulfato de neomicina	20004305006	4
Caelo	Sulfato de neomicina	2003021-02	2
Caelo	Sulfato de neomicina	20E13-F-03	1
Caelo	Sulfato de neomicina	21003216005	14
Caelo	Sulfato de neomicina	21003216006	3
Caelo	Sulfato de neomicina	21003216022	2
Caelo	Sulfato de neomicina	21003216023	1
Caelo	Sulfato de neomicina	21003216025	1
Caelo	Sulfato de neomicina	21003216027	2
Caelo	Sulfato de neomicina	2120520043055	1
Caelo	Sulfato de neomicina	23000856007	1
Caelo	Sulfato de neomicina	24111203	1
Caelo	Sulfato de neomicina	3345	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de neomicina	5/AKD35	1
Caelo	Sulfato de neomicina	5/AKD36	1
Caelo	Sulfato de neomicina	563313062905	1
Caelo	Sulfato de neomicina	8718	1
Caelo	Sulfato de neomicina	9051402	1
Caelo	Sulfato de neomicina	9105316	1
Caelo	Sulfato de neomicina	L34419	1
Caelo	Sulfato de neomicina	N05780	1
Caesar & Loretz GmbH...	Sulfato de neomicina	11/19-N14	1
Caesar & Loretz GmbH...	Sulfato de neomicina	19184903	1
Caesar & Loretz GmbH...	Sulfato de neomicina	20004305005	1
Caesar & Loretz GmbH...	Sulfato de neomicina	20004305005	1
Caesar & Loretz GmbH/Gehe	Sulfato de neomicina	21003216026	1
Caesar & Loretz GmbH...	Sulfato de neomicina	21003216006	3
Caesar & Loretz GmbH...	Sulfato de neomicina	19184903	1
Caesar & Loretz GmbH...	Sulfato de neomicina	18161310	2
Caesar & Loretz GmbH...	Sulfato de neomicina	21003216005	1
Caesar & Loretz GmbH	Sulfato de neomicina	18018704	2
Caesar & Loretz GmbH	Sulfato de neomicina	18161305	2
Caesar & Loretz GmbH	Sulfato de neomicina	18161307	7
Caesar & Loretz GmbH	Sulfato de neomicina	191849001	4
Caesar & Loretz GmbH	Sulfato de neomicina	19184903	10
Caesar & Loretz GmbH	Sulfato de neomicina	20000391004	1
Caesar & Loretz GmbH	Sulfato de neomicina	20004305001	3
Caesar & Loretz GmbH	Sulfato de neomicina	20004305005	6
Caesar & Loretz GmbH	Sulfato de neomicina	20004305006	2
Caesar & Loretz GmbH	Sulfato de neomicina	21003216005	9
Caesar & Loretz GmbH	Sulfato de neomicina	21003216022	1
Caesar & Loretz GmbH	Sulfato de neomicina	21003216026	2
Caesar & Loretz GmbH	Sulfato de neomicina	21003216027	3
Caesar Loretz	Sulfato de neomicina	19184903	1
Caesar&Loretz GmbH,1...	Sulfato de neomicina	16122612	1
Caesar&loretz,AHC,05...	Sulfato de neomicina	15237602	1
caesar&loretz,AHC,7.3.16	Sulfato de neomicina	13062923	1
Caesar&loretz,Phoenix	Sulfato de neomicina	12C13-N04	1
Caesar&Loretz/Noweda	Sulfato de neomicina	15298904	1
Cealo/AHD	Sulfato de neomicina	15J09-B04-314017	1
Cealo	Sulfato de neomicina		1
cealo	Sulfato de neomicina	1502004-03	1
Ebert & Jacobi	Sulfato de neomicina	1601046-01	1
Eur Rho Gehe	Sulfato de neomicina	2003021-01	1
EuRho / Fiebig	Sulfato de neomicina	2003021-02	1
EuRho/Sanacorp	Sulfato de neomicina	1102043-03	1
EuRho/Sanacorp	Sulfato de neomicina	1502004-01	2
EuRho	Sulfato de neomicina	1102043-02	1
EuRho	Sulfato de neomicina	1601046-01	1
Eurho	Sulfato de neomicina	1601046-02	1
EuRho	Sulfato de neomicina	1802005-01	2
euRho	Sulfato de neomicina	1903022-01	1
EuRho	Sulfato de neomicina	2003021-01	2
EuRho	Sulfato de neomicina	2003021-02	1
Euro OTC	Sulfato de neomicina	1102043	2
Euro OTC	Sulfato de neomicina	1102043-01	3
Euro OTC	Sulfato de neomicina	1102043-02	7
Euro OTC	Sulfato de neomicina	1102043-03	4
Euro OTC	Sulfato de neomicina	1303001-03	1
Euro OTC	Sulfato de neomicina	1303033-01	10
Euro OTC	Sulfato de neomicina	1303033-02	15
Euro OTC	Sulfato de neomicina	1303033-03	17
Euro OTC	Sulfato de neomicina	1502004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sulfato de neomicina	1502004-01	19
Euro OTC	Sulfato de neomicina	1502004-02	4
Euro OTC	Sulfato de neomicina	1502004-03	23
Euro OTC	Sulfato de neomicina	151116N	1
Euro OTC	Sulfato de neomicina	1601042	1
Euro OTC	Sulfato de neomicina	1601045-01	2
Euro OTC	Sulfato de neomicina	1601046	1
Euro OTC	Sulfato de neomicina	160104601	3
Euro OTC	Sulfato de neomicina	1601046-01	37
Euro OTC	Sulfato de neomicina	1601046-02	41
Euro OTC	Sulfato de neomicina	1601046-1	1
Euro OTC	Sulfato de neomicina	160146-02	1
Euro OTC	Sulfato de neomicina	16019046-01	1
Euro OTC	Sulfato de neomicina	18020005-01	2
Euro OTC	Sulfato de neomicina	180200501	2
Euro OTC	Sulfato de neomicina	1802005-01	136
Euro OTC	Sulfato de neomicina	1802-005-01	1
Euro OTC	Sulfato de neomicina	180205-01	1
Euro OTC	Sulfato de neomicina	1802095	1
Euro OTC	Sulfato de neomicina	190302-01	1
Euro OTC	Sulfato de neomicina	1903022	3
Euro OTC	Sulfato de neomicina	1903022-01	18
Euro OTC	Sulfato de neomicina	191001209	1
Euro OTC	Sulfato de neomicina	2003021	3
Euro OTC	Sulfato de neomicina	200302101	1
Euro OTC	Sulfato de neomicina	2003021-01	33
Euro OTC	Sulfato de neomicina	200302102	1
Euro OTC	Sulfato de neomicina	2003021-02	63
Euro OTC	Sulfato de neomicina	3021-012	1
Euro OTC	Sulfato de neomicina	3519A-01926	1
Euro OTC	Sulfato de neomicina	G73890	1
Euro OTC	Sulfato de neomicina	L34419	4
Euro OTC	Sulfato de neomicina	N05780	1
Euro OTC	Sulfato de neomicina	w13203	1
Euro OTC	Sulfato de neomicina	W13203	2
euro//Noweda	Sulfato de neomicina	1601046-02	1
Euro/Phönix	Sulfato de neomicina	1502004-01	1
Euro/Phönix	Sulfato de neomicina	1502004-03	1
Euro/Phönix	Sulfato de neomicina	2003021-01	1
Euro/Sanacorp	Sulfato de neomicina	1601046-02	1
Euro/Sanacorp	Sulfato de neomicina	1661046-02	2
Euro/Sanacorp	Sulfato de neomicina	1802005-01	2
Euro/Sanacorp	Sulfato de neomicina	2003021-01	1
euro	Sulfato de neomicina	1502004-02	2
Euroo/Noweda	Sulfato de neomicina	2003021-01	1
Eurp	Sulfato de neomicina	2003021	1
Fagron	Sulfato de neomicina	100810-112-91	1
Fagron	Sulfato de neomicina	10121-N01	1
Fagron	Sulfato de neomicina	11/19-N14	4
Fagron	Sulfato de neomicina	116M-01926	1
Fagron	Sulfato de neomicina	11C21-N10	3
Fagron	Sulfato de neomicina	12C13-N04	4
Fagron	Sulfato de neomicina	12H23-N04	6
Fagron	Sulfato de neomicina	12I19-N14	1
Fagron	Sulfato de neomicina	13D10-N05	5
Fagron	Sulfato de neomicina	13D10-NO5	1
Fagron	Sulfato de neomicina	13G09-N06	1
Fagron	Sulfato de neomicina	13G09N07	2
Fagron	Sulfato de neomicina	13G09-N07	16
Fagron	Sulfato de neomicina	13G09-N070129/340	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de neomicina	13K15-B33-288069	3
Fagron	Sulfato de neomicina	13K15-B33-288073	1
Fagron	Sulfato de neomicina	14A31B02	2
Fagron	Sulfato de neomicina	14A31-B02	2
Fagron	Sulfato de neomicina	14A31B02294696	1
Fagron	Sulfato de neomicina	14A31-B02-294696	5
Fagron	Sulfato de neomicina	14A31-B02-294697	1
Fagron	Sulfato de neomicina	14A31-B02-294698	1
Fagron	Sulfato de neomicina	14A31-B02-296724	1
Fagron	Sulfato de neomicina	14A31-B02-302519	5
Fagron	Sulfato de neomicina	14C27-B05	1
Fagron	Sulfato de neomicina	14c27-B05-302516	1
Fagron	Sulfato de neomicina	14C27-B05-302516	2
Fagron	Sulfato de neomicina	14C27-B05-302517	1
Fagron	Sulfato de neomicina	15/27-B07-321372	2
Fagron	Sulfato de neomicina	1502004-01	2
Fagron	Sulfato de neomicina	1502004-03	1
Fagron	Sulfato de neomicina	15i09-B04-314015	1
Fagron	Sulfato de neomicina	15J09-B04	1
Fagron	Sulfato de neomicina	15j09-b04-314015	1
Fagron	Sulfato de neomicina	15J09-B04314015	1
Fagron	Sulfato de neomicina	15J09-B04-314015	5
Fagron	Sulfato de neomicina	15J09-B04-314017	5
Fagron	Sulfato de neomicina	15J27-B07	1
Fagron	Sulfato de neomicina	15J27-B07-321372	2
Fagron	Sulfato de neomicina	15JO9-B04-314017	1
Fagron	Sulfato de neomicina	16A20-B01-327433	1
Fagron	Sulfato de neomicina	16A20-B10	2
Fagron	Sulfato de neomicina	16A20-B10-324346	2
Fagron	Sulfato de neomicina	16A20-B10-327433	2
Fagron	Sulfato de neomicina	16b10-b50	1
Fagron	Sulfato de neomicina	16B10-B50	3
Fagron	Sulfato de neomicina	16B10-B50-328165	10
Fagron	Sulfato de neomicina	16B28-B05-352957	1
Fagron	Sulfato de neomicina	17B14-B08	1
Fagron	Sulfato de neomicina	17B14-B08-334000	3
Fagron	Sulfato de neomicina	17F12-804	1
Fagron	Sulfato de neomicina	17F12-B04	1
Fagron	Sulfato de neomicina	17f12-b04-340237	1
Fagron	Sulfato de neomicina	17F12-B04-340237	3
Fagron	Sulfato de neomicina	17G05-B04	1
Fagron	Sulfato de neomicina	180200501	1
Fagron	Sulfato de neomicina	1802005-01	6
Fagron	Sulfato de neomicina	183360-0009	1
Fagron	Sulfato de neomicina	18A25-B05-346136	1
Fagron	Sulfato de neomicina	18A25-B05-346138	4
Fagron	Sulfato de neomicina	18A25-B-05-346138	1
Fagron	Sulfato de neomicina	18G28B05	1
Fagron	Sulfato de neomicina	18G28-B05	3
Fagron	Sulfato de neomicina	18g28-b05-352953	1
Fagron	Sulfato de neomicina	18G28-B05-352953	5
Fagron	Sulfato de neomicina	18G28-B05-352957	4
Fagron	Sulfato de neomicina	18G28-B05-354472	7
Fagron	Sulfato de neomicina	19G23-B03	1
Fagron	Sulfato de neomicina	19G23-B03-364716	3
Fagron	Sulfato de neomicina	19G23-B03-364717	1
Fagron	Sulfato de neomicina	19G23-B03-364720	4
Fagron	Sulfato de neomicina	19G23-B03-364717	1
Fagron	Sulfato de neomicina	19G23-B03-364720	1
Fagron	Sulfato de neomicina	19i23-b04-195473	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de neomicina	20A29-F01	1
Fagron	Sulfato de neomicina	20A29-F01-370834	2
Fagron	Sulfato de neomicina	20A29-F01-370836	6
Fagron	Sulfato de neomicina	20A29F01370841	1
Fagron	Sulfato de neomicina	20A29-F01-370841	3
Fagron	Sulfato de neomicina	20A29-F01-370842	1
Fagron	Sulfato de neomicina	20A29-F01-370836	2
Fagron	Sulfato de neomicina	20D08-B07-200574	1
Fagron	Sulfato de neomicina	20do8-b07-200574	1
Fagron	Sulfato de neomicina	20do8-b07-201750	1
Fagron	Sulfato de neomicina	20E13-F03-371373	1
Fagron	Sulfato de neomicina	21D30-F06	2
Fagron	Sulfato de neomicina	21D30-F06-378610	2
Fagron	Sulfato de neomicina	21D30-F06-378614	9
Fagron	Sulfato de neomicina	21D3O-FO6-378614	1
Fagron	Sulfato de neomicina	22E12-B10-224471	1
Fagron	Sulfato de neomicina	23A09-B07-229452	1
Fagron	Sulfato de neomicina	23C10-B04-219531	1
Fagron	Sulfato de neomicina	352954	1
Fagron	Sulfato de neomicina	4312I-01926	1
Fagron	Sulfato de neomicina	b03-364717	1
Fagron	Sulfato de neomicina	F08469	1
Fagron	Sulfato de neomicina	FO8469	1
Fagron	Sulfato de neomicina	M71862	2
Fagron	Sulfato de neomicina	NMZ11006K	1
Fagron	Sulfato de neomicina	X51344	1
Fargon / AHD	Sulfato de neomicina	18G28-B05-354472	1
Fargon	Sulfato de neomicina	15j27-b07-321372	1
fargron	Sulfato de neomicina	14A31-B02-294698	1
Fiebig	Sulfato de neomicina	1502004-03	2
Fragon/Phoenix	Sulfato de neomicina	15J09-B04_322943	1
Gehe 23.11.18	Sulfato de neomicina	1802005-01	1
Gehe Apo-ident	Sulfato de neomicina	200302102	2
GEHE	Sulfato de neomicina	1502001-03	1
Gehe	Sulfato de neomicina	1601046-01	1
Gehe	Sulfato de neomicina	1601046-02	1
GEHE	Sulfato de neomicina	160104602	1
Gehe	Sulfato de neomicina	1802005-01	1
GEHE	Sulfato de neomicina	1802005-01	1
gehe	Sulfato de neomicina	183360-0009	1
Gehe	Sulfato de neomicina	183360-0009	1
Gehe	Sulfato de neomicina	194A-01926	1
Gehe	Sulfato de neomicina	2003021-02	2
Gehe	Sulfato de neomicina	2100321606	1
Gehe	Sulfato de neomicina	23D14-B03-232374	1
Geibo/EuRho	Sulfato de neomicina	180200501	1
Geibo/EuRho	Sulfato de neomicina	1802005-01	1
Hageda	Sulfato de neomicina	1802005-01	1
HenryLamotte	Sulfato de neomicina	1502004-01	1
Jenne	Sulfato de neomicina	15237602	1
Jenne	Sulfato de neomicina	20004305006	1
Jenne	Sulfato de neomicina	GY9146	1
Kehr	Sulfato de neomicina	1601046-02	1
Land/Phönix	Sulfato de neomicina	13062905	2
Nachprüfung	Sulfato de neomicina	2082019-7	1
Noweda/Euro	Sulfato de neomicina		1
Noweda	Sulfato de neomicina	1102043-02	1
Noweda	Sulfato de neomicina	15298902	1
Noweda	Sulfato de neomicina	160104601	1
Noweda	Sulfato de neomicina	1601046-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Sulfato de neomicina	16165016	1
Noweda	Sulfato de neomicina	1802005-01	3
Noweda	Sulfato de neomicina	191849001	1
Noweda	Sulfato de neomicina	20004305001	1
Noweda	Sulfato de neomicina	20A29-F01-370841	1
Noweda	Sulfato de neomicina	23C10-B04-219531	1
Noweda	Sulfato de neomicina	23D14-B03-232374	2
Pfizer USA / Phönix	Sulfato de neomicina	1303033-02	1
Pfizer USA/ Phönix	Sulfato de neomicina	DC3552	1
Pfizer USA/Phoenix	Sulfato de neomicina	2003021-21	1
Pfizer usa	Sulfato de neomicina	160104601	1
Pfizer USA	Sulfato de neomicina	2003021	1
Pfizer USA	Sulfato de neomicina	DC3552	1
Pfizer/Euro OCT Pharma	Sulfato de neomicina	1102043-02	2
Pfizer/Noweda	Sulfato de neomicina	W13203	1
Ph/Euro	Sulfato de neomicina	18020501	1
Pharmacia & Upjohn C...	Sulfato de neomicina	16165017	1
Pharmacia & Upjohn C...	Sulfato de neomicina	16122623	1
phnoix	Sulfato de neomicina	130303301	1
phoenix 13.11.14	Sulfato de neomicina	1303033-03	1
Phoenix	Sulfato de neomicina	1601046-02	2
Phoenix	Sulfato de neomicina	2003021-01	1
Phoenix	Sulfato de neomicina	23000856007	1
Phoenix	Sulfato de neomicina	2400508005	1
Phönix Euro 23.6.21	Sulfato de neomicina	2003021-01	1
Phönix	Sulfato de neomicina	13D10-N05	1
Phönix	Sulfato de neomicina	1601046-02	1
Phönix	Sulfato de neomicina	1802005-01	3
Phönix	Sulfato de neomicina	18A25B05-346138	1
Sanacop/Pharma	Sulfato de neomicina	15J27B07-321372	1
Sanacorp 05.07.2019 5,90EUR	Sulfato de neomicina	18G28-B05-354472	1
Sanacorp/EuRho	Sulfato de neomicina	1601046-01	1
Sanacorp	Sulfato de neomicina	15298902	1
Sanacorp	Sulfato de neomicina	16165016	1
Sanacorp	Sulfato de neomicina	180200501	1
Sanacorp	Sulfato de neomicina	2003021-02	1
Sanacorp	Sulfato de neomicina	23C10-B04-219532	1
Sanacorp	Sulfato de neomicina	23D14-B03-232374	2
Sichuan Long March P...	Sulfato de neomicina	SC-NM-20180109	1
Sichuan Long March P...	Sulfato de neomicina	SC-NM-20190123	3
Sichuan/Noweda	Sulfato de neomicina	SC-NM-20200410	1
siehe WE-Prüfprotokoll	Sulfato de neomicina	19/12	1
Taoasis/Phoenix	Sulfato de neomicina	1502004-01	1
VDL;24.6.14; 3,55EUR	Sulfato de neomicina	1303033-02	2
VDL;9.12;3,55;	Sulfato de neomicina	1303033-03	1

- 234 852 spectra from 1515 *Apo-Ident* customers from a total of 49 022 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de neomicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de neomicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	240	0	201 844
Type C	0	1208	7	234 852

The substance/substance group *Sulfato de neomicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	99.4239 % (> 99.1770 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21771	21771	0,00	113,96
21814	21814	0,00	121,41
21894	21894	0,00	91,71
21961	21814	19,92	119,25
22276	21814	3,44	121,12
22381	22381	0,00	130,86
23856	23856	0,00	76,22
25185	22381	8,40	139,76
25643	25643	0,00	112,36
26286	21771	10,62	118,13
26664	22381	15,16	141,16
27052	22381	28,14	95,61
27222	27222	0,00	92,18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de polimixina B**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20853-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de polimixina B; Polimixina B, sulfato; Polymyxini B sulfas

Special notes

When selecting the *Sulfato de polimixina B* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de polimixina B	14	14	80

Second-stage model

For differentiation of the substance/substance group *Sulfato de polimixina B* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de polimixina B* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de colistina	40,74	18,66
Bacitracina	46,53	19,73
Pantotenato de cálcio	60,05	19,84
⋮	⋮	⋮
Riboflavina	>50	33,80
Anfotericina B	>50	41,16
Nistatina	>50	52,81
Cianocobalamina	>50	56,42
Triancinolona	>50	62,28
Metilcobalamina	>50	65,85
Vitamina E acetato pó 50%	>50	75,82
Glicerofosfato de cálcio	>50	77,34
Gelatina, branca	>50	79,09
Levedura de selênio	>50	84,03
Estradiol hemi-hidratado	>50	86,68
Estriol	>50	90,55
Bromidrato de hioscina	>50	100,16
Carmelose sódica	>50	119,76
Tosilcloramida sódica	>50	120,97
SyrSpend® SF Alka	>50	136,66
SyrSpend® SF pH4 neo	>50	159,66
Amido de arroz	>50	166,04
Ácido oxálico	>50	236,51
Amido de milho	>50	243,23
Goma arábica, dispersão seca	>50	261,59
SyrSpend® SF pH4	>50	286,90
Fécula de batata	>50	339,84
Amido de trigo	>50	347,00
Maltodextrina	>50	373,01
Frutose	>50	395,71

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de polimixina B* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de polimixina B*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de polimixina B	153501	22451	60	20160318*
Caelo	Sulfato de polimixina B	181154	24407	40	20180507*
Euro OTC	Sulfato de polimixina B	1304033-01	21094	40	20130829
Euro OTC	Sulfato de polimixina B	1202039-02	21329	40	1411033
Euro OTC	Sulfato de polimixina B	1304033-02	21584	60	20130612
Euro OTC	Sulfato de polimixina B	1505005-01	21980	60	AR-16-FG-005387-01
Euro OTC	Sulfato de polimixina B	1604016	22542	40	20160509*
Euro OTC	Sulfato de polimixina B	2101014	25597	40	20210331*
Euro OTC	Sulfato de polimixina B	2303014	26763	40	20230525*
Fagron	Sulfato de polimixina B	13C12-N02	20853	40	1402691
Fagron	Sulfato de polimixina B	12G13-N05	21258	40	1410347
Fagron	Sulfato de polimixina B	13I13-N05	21595	45	AR-15-FG-001516-01
Fagron	Sulfato de polimixina B	14F04-B03-296722	21957	60	20140708
Fagron	Sulfato de polimixina B	15H14-B01-314364	22323	60	20150902

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 665 spectra of 14 reference samples from the substance/substance group *Sulfato de polimixina B*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.
- 152 297 spectra from a total of 2828 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 660 spectra of 18 reference samples from the substance/substance group *Sulfato de polimixina B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de polimixina B	191131	24752	40
Caelo	Sulfato de polimixina B	22001497	26255	40
Caelo	Sulfato de polimixina B	23001927	26970	40
Euro OTC	Sulfato de polimixina B	1701010	23012	40
Euro OTC	Sulfato de polimixina B	1707013	23554	40
Euro OTC	Sulfato de polimixina B	1802006	23953	40
Euro OTC	Sulfato de polimixina B	1807004	24143	40
Euro OTC	Sulfato de polimixina B	1811022	24494	40
Euro OTC	Sulfato de polimixina B	1906002	24779	40
Euro OTC	Sulfato de polimixina B	1911021	25088	40
Euro OTC	Sulfato de polimixina B	2006009	25317	40
Euro OTC	Sulfato de polimixina B	2205005	26226	40
Fagron	Sulfato de polimixina B	13E06-N12	20912	40
Fagron	Sulfato de polimixina B	22A21-B03-218149	26144	40
Caelo	Sulfato de polimixina B	22001497	26255SI	20
Euro OTC	Sulfato de polimixina B	1202039-02	20904	40
Euro OTC	Sulfato de polimixina B	2205005	26226SI	20
Fagron	Sulfato de polimixina B	22A21-B03-218149	26144SI	20

- 201 424 spectra from a total of 4030 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 248 spectra from 161 *Apo-Ident* customers from 86 batches from the substance/substance group *Sulfato de polimixina B*.

- Among them are spectra of independent samples from 80 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de polimixina B	2101014-01	1
	Sulfato de polimixina B	22K22-B02-224472	1
	Sulfato de polimixina B	230035622001	1
	Sulfato de polimixina B	2303014-01	2
	Sulfato de polimixina B	230314-01	1
Alliance Healthcare	Sulfato de polimixina B	1202039-02	1
apo-ident/Gehe/24,50	Sulfato de polimixina B	1807004-01	1
Biotika / Ebert	Sulfato de polimixina B	15011	1
Biotika a.s./Phoenix	Sulfato de polimixina B	2101014-01	1
Biotika/Noweda	Sulfato de polimixina B	200317	1
Biotika	Sulfato de polimixina B	150828	1
Bombastus	Sulfato de polimixina B	1604016-02	1
Caelo	Sulfato de polimixina B	1102013-01	1
Caelo	Sulfato de polimixina B	12G13-N05	3
Caelo	Sulfato de polimixina B	13H28-B02-287953	1
Caelo	Sulfato de polimixina B	150725	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de polimixina B	15350101	8
Caelo	Sulfato de polimixina B	15350101P-190311-3	1
Caelo	Sulfato de polimixina B	1604016-01	3
Caelo	Sulfato de polimixina B	16C01-B04-319432	1
Caelo	Sulfato de polimixina B	170101001	3
Caelo	Sulfato de polimixina B	1701010-01	1
Caelo	Sulfato de polimixina B	1707013-01	1
Caelo	Sulfato de polimixina B	1802006-01	2
Caelo	Sulfato de polimixina B	1802006-011	1
Caelo	Sulfato de polimixina B	18115406	2
Caelo	Sulfato de polimixina B	18115410	2
Caelo	Sulfato de polimixina B	19113102	1
Caelo	Sulfato de polimixina B	19113103	1
Caelo	Sulfato de polimixina B	20003057003	3
Caesar & Loretz GmbH	Sulfato de polimixina B	20003057003	2
cealo	Sulfato de polimixina B	16c01-b04-319432	1
EuRho/Phoenix	Sulfato de polimixina B	2006009-01	1
EuRho	Sulfato de polimixina B	1202039-01	1
EuRho	Sulfato de polimixina B	1807004-01	1
EuRho	Sulfato de polimixina B	2006008-01	1
Euro OTC	Sulfato de polimixina B	11091419	1
Euro OTC	Sulfato de polimixina B	1202039-01	1
Euro OTC	Sulfato de polimixina B	1202039-02	4
Euro OTC	Sulfato de polimixina B	1304033-01	1
Euro OTC	Sulfato de polimixina B	1304033-02	1
Euro OTC	Sulfato de polimixina B	1304033-03	2
Euro OTC	Sulfato de polimixina B	1406012-01	3
Euro OTC	Sulfato de polimixina B	140601202	3
Euro OTC	Sulfato de polimixina B	1406012-02	5
Euro OTC	Sulfato de polimixina B	150500501	1
Euro OTC	Sulfato de polimixina B	1505005-01	6
Euro OTC	Sulfato de polimixina B	1505505-01	1
Euro OTC	Sulfato de polimixina B	1604016-01	2
Euro OTC	Sulfato de polimixina B	1604016-02	6
Euro OTC	Sulfato de polimixina B	170101001	1
Euro OTC	Sulfato de polimixina B	1701010-01	13
Euro OTC	Sulfato de polimixina B	1707013-01	10
Euro OTC	Sulfato de polimixina B	180200601	1
Euro OTC	Sulfato de polimixina B	1802006-01	8
Euro OTC	Sulfato de polimixina B	1807004-01	6
Euro OTC	Sulfato de polimixina B	1811022-01	7
Euro OTC	Sulfato de polimixina B	1906002-01	6
Euro OTC	Sulfato de polimixina B	1911021-01	5
Euro OTC	Sulfato de polimixina B	2006009-01	15
Euro OTC	Sulfato de polimixina B	2101014-01	21
Euro OTC	Sulfato de polimixina B	2205005-01	1
Euro OTC	Sulfato de polimixina B	23051502	1
Euro OTC	Sulfato de polimixina B	25101201	1
Euro OTC	Sulfato de polimixina B	28041730	1
Euroo/Phoenix	Sulfato de polimixina B	1304033-02	1
Fagron	Sulfato de polimixina B	12G13N05	1
Fagron	Sulfato de polimixina B	12G13-N05	1
Fagron	Sulfato de polimixina B	13/13-N05	1
Fagron	Sulfato de polimixina B	13G05-N06	2
Fagron	Sulfato de polimixina B	13H28-B02-287954	1
Fagron	Sulfato de polimixina B	13H28-B02-293470	1
Fagron	Sulfato de polimixina B	140822	1
Fagron	Sulfato de polimixina B	14F04-B03-296721	1
Fagron	Sulfato de polimixina B	14H12-B06-304727	1
Fagron	Sulfato de polimixina B	15H14-B01-315692	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de polimixina B	16C01-B04	1
Fagron	Sulfato de polimixina B	16C01-B04-319432	1
Fagron	Sulfato de polimixina B	16c01b04322012	1
Fagron	Sulfato de polimixina B	16C01-B04-322012	3
Fagron	Sulfato de polimixina B	16G21-B03-333808	1
Fagron	Sulfato de polimixina B	170621	1
Fagron	Sulfato de polimixina B	17H23-B01-344840	2
Fagron	Sulfato de polimixina B	18B28B04351511	1
Fagron	Sulfato de polimixina B	18B28-B04-355722	2
Fagron	Sulfato de polimixina B	19/11-F01-368351	1
Fagron	Sulfato de polimixina B	191057	1
Fagron	Sulfato de polimixina B	19A23-B01-361158	4
Fagron	Sulfato de polimixina B	19A23-B01-3621201	1
Fagron	Sulfato de polimixina B	19A23-B01-362121	2
Fagron	Sulfato de polimixina B	19I11-F01-3683501	1
Fagron	Sulfato de polimixina B	20B21-F08-373930	1
Fagron	Sulfato de polimixina B	20F23-F01	1
Fagron	Sulfato de polimixina B	21K09-B10-213615	1
Fagron	Sulfato de polimixina B	22A21-B03-218149	1
Fagron	Sulfato de polimixina B	2517M-03315	1
Fagron	Sulfato de polimixina B	3518A-03315	1
Fagron	Sulfato de polimixina B	912A-03315	1
Fagron	Sulfato de polimixina B	F08-3739300	1
Fargon/Phoenix	Sulfato de polimixina B	17H23-B01-344840	1
Fiebig	Sulfato de polimixina B	1807004-01	1
Gatt-Koller	Sulfato de polimixina B	17H23B01344840	1
Gehe	Sulfato de polimixina B	170101001	1
GEHE	Sulfato de polimixina B	1701010-01	1
Noweda 03.08.2019	Sulfato de polimixina B	18115406	1
Phoenix	Sulfato de polimixina B	1807004-01	1
Phoenix	Sulfato de polimixina B	2006009-01	1
Phönix/Euro	Sulfato de polimixina B	1505005-010	1
Phönix	Sulfato de polimixina B	1202039-01	1
Phönix	Sulfato de polimixina B	1701010-01	1
Phönix	Sulfato de polimixina B	1707013	1
Rondell Apotheke	Sulfato de polimixina B	121161	1
Sanacorp	Sulfato de polimixina B	1707013-01	1
Sanacorp	Sulfato de polimixina B	2101014-01	1

- 235 819 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de polimixina B* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de polimixina B* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	665	0	152 297
Type B	0	660	0	201 424
Type C	0	244	4	235 819

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Sulfato de polimixina B* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0977 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0909 %)
Type C	100.0000 % (> 99.9007 %)	98.3871 % (> 97.1774 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20853	20853	0,00	49,22
21094	21980	7,02	55,80
21258	21258	0,00	48,52
21329	21329	0,00	51,58
21584	21980	13,37	57,97
21595	21595	0,00	65,96
21957	22451	4,74	62,77
21980	21980	0,00	57,87
22323	25597	8,21	61,24
22451	22451	0,00	66,25
22542	22542	0,00	49,29
24407	24407	0,00	46,53
25597	25597	0,00	59,91
26763	26763	0,00	55,61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de quinidina di-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20819-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de quinidina di-hidratado; Chinidini sulfas; Quinidina, sulfato di-hidratado

Special notes

When selecting the *Sulfato de quinidina di-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de quinidina di-hidratado	6	4	5

Second-stage model

For differentiation of the substance/substance group *Sulfato de quinidina di-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de quinidina di-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	91,17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de quinidina di-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de quinidina di-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulfato de quinidina di-h…	12L04-N10	20819	40	AR-14-FG-013249-01
Fagron	Sulfato de quinidina di-h…	12J16-B03	21217	39	1412323
Fagron	Sulfato de quinidina di-h…	14I04-B09-304357	21810	60	AR-15-FG-015409-01
Fagron	Sulfato de quinidina di-h…	22A17-B09-222135	26331	40	20220304
Fagron	Sulfato de quinidina di-h…	22A17-B09-222135	26331SI	20	20220304
Fagron	Sulfato de quinidina di-h…	23E17-B03-230370	26903	40	20230605
Fagron	Sulfato de quinidina di-h…	24E08-B13-001927	27408	40	20240705

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 279 spectra of 7 reference samples from the substance/substance group *Sulfato de quinidina di-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 683 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Sulfato de quinidina di-hidratado*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Sulfato de quinidina di-h…	16A06-B04-324954	22970	40
Fagron	Sulfato de quinidina di-h…	18B01-B08-350965	24181	40
Fagron	Sulfato de quinidina di-h…	20C23-F02-373172	25485	40
Fagron	Sulfato de quinidina di-h…	21E06-B01-213612	25901	40
Fagron	Sulfato de quinidina di-h…	21E06-B01-213612	25901SI	10
Fagron	Sulfato de quinidina di-h…	23E17-B03-230370	26903SI†	20

- 201 894 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Sulfato de quinidina di-hidratado*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
buchler GmbH	Sulfato de quinidina di-h…	16a06-b04-340797	1
Caelo	Sulfato de quinidina di-h…	16A06-B04-330856	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de quinidina di-h…	13G08-N02	1
Fagron	Sulfato de quinidina di-h…	18B01-B08-356315	1
Fagron	Sulfato de quinidina di-h…	21E06-B01-213612	1

- 236 062 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de quinidina di-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de quinidina di-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	279	0	152 683
Type B	0	190	0	201 894
Type C	0	5	0	236 062

The substance/substance group *Sulfato de quinidina di-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8495 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20819	20819	0,00	191,09
21217	21217	0,00	191,36
21810	21810	0,00	190,89

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26331	21810	9,50	191,38
26903	21810	4,35	193,39
27408	21810	8,86	191,22

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de quinina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21057-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de quinina; Chinini sulfas; Quinina, sulfato

Special notes

When selecting the *Sulfato de quinina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de quinina	6	2	6

Second-stage model

For differentiation of the substance/substance group *Sulfato de quinina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de quinina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	101,73	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de quinina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de quinina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de quinina	13024604	21429	60	AR-16-FG-005472-01
Caelo	Sulfato de quinina	15230005	22959	40	20150729
Fagron	Sulfato de quinina	13J23-N03	21057	40	1404401
Fagron	Sulfato de quinina	14B27-B01	21277	40	AR-16-FG-009455-01
Fagron	Sulfato de quinina	22B24-B03-216222	26143	40	20220423
Fagron	Sulfato de quinina	22B24-B03-216222	26143SI	20	20220423
Fagron	Sulfato de quinina	23C09-B03-229466	26681	40	20230327
Fagron	Sulfato de quinina	23C09-B03-229466	26681SI	20	20230327

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 8 reference samples from the substance/substance group *Sulfato de quinina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 662 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sulfato de quinina*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de quinina	170616	23281	40
Caelo	Sulfato de quinina	180630	24032	40
Caelo	Sulfato de quinina	170616	23316	40

- 201 964 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Sulfato de quinina*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de quinina	15B06B03304359	1
Gatt-Koller / Phoenix	Sulfato de quinina	2503/07143314	1
Gatt-Koller / Phoenix	Sulfato de quinina	4928/11132214	1
Gatt-Koller	Sulfato de quinina	1801042	1
Gatt-Koller	Sulfato de quinina	1803149	4
KÖGL	Sulfato de quinina	1901102	1

- 236 058 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de quinina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de quinina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	120	0	201 964
Type C	0	8	1	236 058

The substance/substance group *Sulfato de quinina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21057	21057	0,00	177,65
21277	21277	0,00	173,40
21429	21429	0,00	177,23
22959	21429	9,69	173,27
26143	21277	7,39	167,57
26681	21057	10,48	171,51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de salbutamol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20476-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de salbutamol; Salbutamol, sulfato; Salbutamoli sulfas

Special notes

When selecting the *Sulfato de salbutamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de salbutamol	4	1	0

Second-stage model

For differentiation of the substance/substance group *Sulfato de salbutamol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de salbutamol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	80,45	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de salbutamol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de salbutamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulfato de salbutamol	13K12-N02	23232	40	1801521
Fagron	Sulfato de salbutamol	17I21-B02	23993	40	20170311
Fagron	Sulfato de salbutamol	22C07-B04-222382	26466	40	20220613
Fagron	Sulfato de salbutamol	23H24-B03-231712	27038	40	20231116
Fagron	Sulfato de salbutamol	23H24-B03-231712	27038SI	20	20231116

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Sulfato de salbutamol*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 782 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 8 reference samples from the substance/substance group *Sulfato de salbutamol*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Sulfato de salbutamol	18H21-B03-364945	26077	40
Fagron	Sulfato de salbutamol	13K12-N02	21691	60
Fagron	Sulfato de salbutamol	13K12-N02	23231	40
Fagron	Sulfato de salbutamol	13K12-N02	23454	40
Fagron	Sulfato de salbutamol	13K12-N02	23455	40
Fagron	Sulfato de salbutamol	13K12-N02	23755	40
Fagron	Sulfato de salbutamol	13K12-N02	23756	40
Fagron	Sulfato de salbutamol	18H21-B03-364945	26077SI	20

- 201 764 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Sulfato de salbutamol*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Noweda	Sulfato de salbutamol	13K12-N02	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de salbutamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de salbutamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	320	0	201 764
Type C	0	1	0	236 066

The substance/substance group *Sulfato de salbutamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23232	23232	0,00	260,02
23993	23232	42,86	257,56
26466	23232	38,67	265,54
27038	23232	37,12	267,38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de sódio deca-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20124-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de sódio deca-hidratado; Natrii sulfas decahydricus

Special notes

When selecting the *Sulfato de sódio deca-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de sódio deca-hidratado	2	2	29

Second-stage model

For differentiation of the substance/substance group *Sulfato de sódio deca-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de sódio deca-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	81,39	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de sódio deca-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de sódio deca-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfato de sódio deca-hid…	23001158	27082	40	20230609*
Caelo	Sulfato de sódio deca-hid…	23001158	27082SI	20	20230609*
Euro OTC	Sulfato de sódio deca-hid…	2111018	26149	40	20211126*
Euro OTC	Sulfato de sódio deca-hid…	2111018	26149SI	20	20211126*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 4 reference samples from the substance/substance group *Sulfato de sódio deca-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 842 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 3 reference samples from the substance/substance group *Sulfato de sódio deca-hidratado*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sulfato de sódio deca-hid…	1708012-02	24274	40
Euro OTC	Sulfato de sódio deca-hid…	2301001	27086	40
Euro OTC	Sulfato de sódio deca-hid…	2301001	27086SI	20

- 201 984 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 73 spectra from 29 *Apo-Ident* customers from 29 batches from the substance/substance group *Sulfato de sódio deca-hidratado*.

- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caaelo	Sulfato de sódio deca-hid…	11294603	2
Caelo	Sulfato de sódio deca-hid…	11012207	1
Caelo	Sulfato de sódio deca-hid…	11012210	2
Caelo	Sulfato de sódio deca-hid…	12157001	1
Caelo	Sulfato de sódio deca-hid…	12157005	13
Caelo	Sulfato de sódio deca-hid…	12157006	3
Caelo	Sulfato de sódio deca-hid…	12157007	1
Caelo	Sulfato de sódio deca-hid…	12157011	1
Caelo	Sulfato de sódio deca-hid…	12157012	18

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de sódio deca-hid…	12157013	1
Caelo	Sulfato de sódio deca-hid…	12256902	1
Caelo	Sulfato de sódio deca-hid…	12257901	1
Caelo	Sulfato de sódio deca-hid…	12257902	5
Caelo	Sulfato de sódio deca-hid…	18101202	1
Caelo	Sulfato de sódio deca-hid…	205026	1
Caelo	Sulfato de sódio deca-hid…	61599506	1
Caelo	Sulfato de sódio deca-hid…	70706387	1
EuRho	Sulfato de sódio deca-hid…	1210005-01	1
Euro OTC	Sulfato de sódio deca-hid…	1108035-01	3
Euro OTC	Sulfato de sódio deca-hid…	1108035-02	2
Euro OTC	Sulfato de sódio deca-hid…	121000502	2
Euro OTC	Sulfato de sódio deca-hid…	1210005-02	2
Euro OTC	Sulfato de sódio deca-hid…	4312I-01920	1
Fagron	Sulfato de sódio deca-hid…	1464	1
Fagron	Sulfato de sódio deca-hid…	2134	1
fargon/Sanacorp	Sulfato de sódio deca-hid…	12H31-N04	1
Fiebig 29.04.13 ek: 5,64EUR	Sulfato de sódio deca-hid…	1210005-01	1
Gehe	Sulfato de sódio deca-hid…	12257902	1
Hedinger/Phönix	Sulfato de sódio deca-hid…	205025	1
nachprüfung	Sulfato de sódio deca-hid…	C1069	1
Unisan	Sulfato de sódio deca-hid…	11294605	1

- 235 994 spectra from 1515 *Apo-Ident* customers from a total of 49 229 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de sódio deca-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de sódio deca-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	100	0	201 984
Type C	0	73	0	235 994

The substance/substance group *Sulfato de sódio deca-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.7808 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26149	26149	0,00	156,16
27082	27082	0,00	166,48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de tobramicina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20951-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de tobramicina; Tobramicina, sulfato; Tobramycini sulfas

Special notes

When selecting the *Sulfato de tobramicina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de tobramicina	15	4	19

Second-stage model

For differentiation of the substance/substance group *Sulfato de tobramicina* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de tobramicina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de neomicina	20,71	15,61
Sulfato de polimixina B	52,33	–
⋮	⋮	⋮
Fosfato sódico de riboflavina hidratado	>50	69,59
Fosfato de Mg-Ca-K-colamina	>50	75,74
Gluconato de zinco	>50	87,49
Carbômero	>50	109,21
Sulfato de gentamicina	>50	127,63
Citrato de magnésio	>50	134,93
Tetraborato de sódio	>50	473,95
Finasterida	>50	1421,13

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de tobramicina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de tobramicina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Sulfato de tobramicina	AP15061047002T	22393	40	1608462
Audor Pharma	Sulfato de tobramicina	AP15061047002T	23502	40	20160322
Euro OTC	Sulfato de tobramicina	1301011-02	21624	60	1508071
Euro OTC	Sulfato de tobramicina	1505015-01	21832	60	8963
Euro OTC	Sulfato de tobramicina	1510035-01	22240	60	9202
Euro OTC	Sulfato de tobramicina	1510035	22252	60	20151208*
Euro OTC	Sulfato de tobramicina	1807045	24321	40	20180917*
Euro OTC	Sulfato de tobramicina	2001010	25100	40	20200113*
Euro OTC	Sulfato de tobramicina	2202013	26045	40	20220324*
Euro OTC	Sulfato de tobramicina	2404002	27371	40	20240904*
Fagron	Sulfato de tobramicina	12G03-N03	20951	40	1404541

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulfato de tobramicina	15I17-B04-315697	22359	45	20150928
Fagron	Sulfato de tobramicina	16B05-B03-336397	23515	40	1801385
Fagron	Sulfato de tobramicina	20H13-F05-373631	25506	40	2105375
Fagron	Sulfato de tobramicina	20F18-F05-376114	25507	40	2105376
Fagron	Sulfato de tobramicina	23K07-B16-233773	27050	40	20231215
Fagron	Sulfato de tobramicina	23K07-B16-233773	27050SI	20	20231215

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 745 spectra of 17 reference samples from the substance/substance group *Sulfato de tobramicina*. These samples are listed above in the *calibration samples* section. The reference samples come from 15 different batches.

- 152 217 spectra from a total of 2827 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Sulfato de tobramicina*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sulfato de tobramicina	1710029	23870	40
Euro OTC	Sulfato de tobramicina	1910008	25085	40
Euro OTC	Sulfato de tobramicina	2211003	26569	40
Fagron	Sulfato de tobramicina	20A14-F02-368920	25184	40
Euro OTC	Sulfato de tobramicina	2202013	26045SI†	10
Euro OTC	Sulfato de tobramicina	2211003	26569SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 894 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 33 spectra from 14 *Apo-Ident* customers from 22 batches from the substance/substance group *Sulfato de tobramicina*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sulfato de tobramicina	22E06-B02-224488	2
	Sulfato de tobramicina	B02-2283406	1
EuRho/VDL01	Sulfato de tobramicina	1710029-01	1
Euro OCT/Noweda	Sulfato de tobramicina	1510035-01	1
Euro OTC	Sulfato de tobramicina	1505015-01	1
Euro OTC	Sulfato de tobramicina	15I17-B04-315697	1
Euro OTC	Sulfato de tobramicina	1807045-01	3
Fagron	Sulfato de tobramicina	13H09-N09	1
Fagron	Sulfato de tobramicina	15/17-B04-315697	1
Fagron	Sulfato de tobramicina	16b-03-319433	1
Fagron	Sulfato de tobramicina	16B05-B03	4
Fagron	Sulfato de tobramicina	16B05-B03-317988	2
Fagron	Sulfato de tobramicina	16B05-B03-319433	1
Fagron	Sulfato de tobramicina	16B05-B03-330974	2
Fagron	Sulfato de tobramicina	17E05-B03-338122	2
Fagron	Sulfato de tobramicina	17J12-B04-341324	2
Fagron	Sulfato de tobramicina	20A14-F02-368920	2
Fagron	Sulfato de tobramicina	20H13-F05-373633	1
Fagron	Sulfato de tobramicina	21A04-F02	1
Fagron	Sulfato de tobramicina	21H30-B02-213664	1
Fagron	Sulfato de tobramicina	21H30-B02-213666	1
PHOENIX 31.01.2014	Sulfato de tobramicina	1202006-01	1

- 236 034 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de tobramicina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de tobramicina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	745	0	152 217
Type B	0	190	0	201 894
Type C	0	32	1	236 034

The substance/substance group *Sulfato de tobramicina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1946 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	96.9697 % (> 87.8788 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20951	20951	0,00	112,32
21624	21624	0,00	95,71
21832	21832	0,00	89,63
22240	22240	0,00	121,91
22252	22252	0,00	89,69
22359	23515	20,29	102,22
22393	22393	0,00	55,55
23502	25100	15,64	69,86
23515	23515	0,00	99,21
24321	24321	0,00	70,01
25100	25100	0,00	84,36
25506	25506	0,00	173,42
25507	25507	0,00	164,12
26045	26045	0,00	105,60
27050	22240	33,45	159,61
27371	27371	0,00	54,59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfato de zinco hepta-hidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10006391-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfato de zinco hepta-hidratado; Zinci sulfas heptahydricus

Special notes

When selecting the *Sulfato de zinco hepta-hidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfato de zinco hepta-hidratado	2	2	13

Second-stage model

For differentiation of the substance/substance group *Sulfato de zinco hepta-hidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfato de zinco hepta-hidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de magnésio hepta-hidratado	24,75	–
Cromoglicato de sódio	60,55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfato de zinco hepta-hidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfato de zinco hepta-hidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Sulfato de zinco hepta-hi…	2206010	26554	40	20220624*
Euro OTC	Sulfato de zinco hepta-hi…	2206010	26554SI	20	20220624*
Euro OTC	Sulfato de zinco hepta-hi…	2210021	26555	40	20221122*
Euro OTC	Sulfato de zinco hepta-hi…	2210021	26555SI	20	20221122*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 4 reference samples from the substance/substance group *Sulfato de zinco hepta-hidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 842 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 2 reference samples from the substance/substance group *Sulfato de zinco hepta-hidratado*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfato de zinco hepta-hi…	23002587	27077	40
Euro OTC	Sulfato de zinco hepta-hi…	2107023	25788	50

- 201 994 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 14 spectra from 10 *Apo-Ident* customers from 13 batches from the substance/substance group *Sulfato de zinco hepta-hidratado*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de zinco hepta-hi…	11095601	1
Caelo	Sulfato de zinco hepta-hi…	11095621	1
Caelo	Sulfato de zinco hepta-hi…	12257802	1
Caelo	Sulfato de zinco hepta-hi…	12257809	2
Caelo	Sulfato de zinco hepta-hi…	12257816	1
Caelo	Sulfato de zinco hepta-hi…	12257818	1
Caelo	Sulfato de zinco hepta-hi…	4012Q-02798	1
Caelo	Sulfato de zinco hepta-hi…	81554199	1
Euro OTC	Sulfato de zinco hepta-hi…	1105002-01	1
Euro OTC	Sulfato de zinco hepta-hi…	1201031-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sulfato de zinco hepta-hi…	1201031-02	1
Euro OTC	Sulfato de zinco hepta-hi…	1201031-2	1
Euro OTC	Sulfato de zinco hepta-hi…	1309011_0	1

- 236 053 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfato de zinco hepta-hidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfato de zinco hepta-hidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	90	0	201 994
Type C	0	14	0	236 053

The substance/substance group *Sulfato de zinco hepta-hidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26554	26554	0,00	75,81
26555	26555	0,00	44,10

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfoguaiacolato de potássio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20327-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfoguaiacolato de potássio; Sulfoguaiacolum hydricum

Special notes

When selecting the *Sulfoguaiacolato de potássio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfoguaiacolato de potássio	6	2	1

Second-stage model

For differentiation of the substance/substance group *Sulfoguaiacolato de potássio* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfoguaiacolato de potássio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	71,83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfoguaiacolato de potássio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfoguaiacolato de potássio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfoguaiacolato de potássio	13405805	21696	45	20140108
Caelo	Sulfoguaiacolato de potássio	190303	24495	40	20190222*
Caelo	Sulfoguaiacolato de potássio	20001657	25191	40	20200619*
Gatt-Koller	Sulfoguaiacolato de potássio	1156/04152115	21843	60	20150410
Gatt-Koller	Sulfoguaiacolato de potássio	4543/01170317	23113	40	AR-17-FG-012520-01
Gatt-Koller	Sulfoguaiacolato de potássio	23J00290	26680	40	20230314
Gatt-Koller	Sulfoguaiacolato de potássio	23J00290	26680SI	20	20230314

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 285 spectra of 7 reference samples from the substance/substance group *Sulfoguaiacolato de potássio*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 677 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sulfoguaiacolato de potássio*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfoguaiacolato de potássio	170919	23300	40
Caelo	Sulfoguaiacolato de potássio	190921	24732	40
Caelo	Sulfoguaiacolato de potássio	170919	23306	40

- 201 964 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Sulfoguaiacolato de potássio*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sulfoguaiacolato de potássio	15343912	12

- 236 055 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfoguaiacolato de potássio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfoguaiacolato de potássio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	285	0	152 677
Type B	0	120	0	201 964
Type C	0	12	0	236 055

The substance/substance group *Sulfoguaiacolato de potássio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8947 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21696	23113	22,13	203,29
21843	23113	26,71	198,83
23113	23113	0,00	213,28
24495	24495	0,00	207,22
25191	25191	0,00	221,38
26680	25191	25,76	214,01

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulpirida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005288-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulpirida; Sulpiridum

Special notes

When selecting the *Sulpirida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulpirida	2	3	0

Second-stage model

For differentiation of the substance/substance group *Sulpirida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulpirida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	151,54	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulpirida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulpirida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulpirida	20I16-F01-374539	26320	40	230502387
Fagron	Sulpirida	20I16-F01-374539	26320SI	20	230502387
Pharma Che…	Sulpirida	21F16-1226	26318	40	20210616
Pharma Che…	Sulpirida	21F16-1226	26318SI	20	20210616

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 4 reference samples from the substance/substance group *Sulpirida*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 842 spectra from a total of 2840 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Sulpirida*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Sulpirida	18H09-B08-355949	25692	50
FSA Chemicals	Sulpirida	19G29-APR90102	25693	50
FSA Chemicals	Sulpirida	21G16-APR21165	26319	40
FSA Chemicals	Sulpirida	21G16-APR21165	26319SI	20

- 201 924 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sulpirida*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulpirida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulpirida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	160	0	201 924
Type C	0	0	0	236 067

The substance/substance group *Sulpirida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26318	26320	36,13	236,06
26320	26320	0,00	236,60

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tacrolimo monoidratado**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	10005936-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tacrolimo monoidratado; Tacrolimusum monohydricum

Special notes

When selecting the *Tacrolimo monoidratado* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tacrolimo monoidratado	4	3	1

Second-stage model

For differentiation of the substance/substance group *Tacrolimo monoidratado* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tacrolimo monoidratado* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	99,09	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tacrolimo monoidratado* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tacrolimo monoidratado*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tacrolimo monoidratado	2201007	25941	40	20220301*
Euro OTC	Tacrolimo monoidratado	2205032	26417	30	20221110*
Fagron	Tacrolimo monoidratado	21I24-B12-215778	26147	40	20211223
Fagron	Tacrolimo monoidratado	21I24-B12-215778	26147SI	20	20211223
Fagron	Tacrolimo monoidratado	23K23-B05-223469	27048	40	20231229

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 170 spectra of 5 reference samples from the substance/substance group *Tacrolimo monoidratado*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 792 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Tacrolimo monoidratado*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tacrolimo monoidratado	1904015	24605	40
Euro OTC	Tacrolimo monoidratado	2304013	26762	40
Euro OTC	Tacrolimo monoidratado	2405003	27360	40
Euro OTC	Tacrolimo monoidratado	2201007	25941SI†	10
Euro OTC	Tacrolimo monoidratado	2304013	26762SI	20

- 201 934 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Tacrolimo monoidratado*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tacrolimo monoidratado	2304013-01	2
Euro OTC	Tacrolimo monoidratado	2304013-01	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tacrolimo monoidratado* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tacrolimo monoidratado* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	170	0	152 792
Type B	0	150	0	201 934
Type C	0	3	0	236 064

The substance/substance group *Tacrolimo monoidratado* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.4706 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25941	25941	0,00	146,02
26147	25941	20,68	149,00
26417	26417	0,00	150,16
27048	26417	21,25	150,85

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tanino**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20018-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tanino; Tanninum

Special notes

When selecting the *Tanino* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tanino	6	3	154

Second-stage model

For differentiation of the substance/substance group *Tanino* the following second-stage model is used:

- Submodelo 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tanino* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	54,53	–
⋮	⋮	⋮
Cloreto de dequalínio	>50	48,63
Cloridrato de oxitetraciclina	>50	72,35
Levotiroxina sódica	>50	95,27
Eosina amarela	>50	95,87
Ditranol	>50	489,15
Ácido acetilsalicílico	>50	539,60
Salicilato de sódio	>50	709,01
Ácido benzoico	>50	1074,05

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tanino* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tanino*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tanino	12336016	21608	60	20121127
Caelo	Tanino	172092	23631	40	20170829*
Caelo	Tanino	20002512002	25516	40	20200904
Caelo	Tanino	22001643	26254	40	20220613*
Fagron	Tanino	13H30-B03-287645	21653	60	1711482
Fagron	Tanino	16D08-B04-328410	23211	40	AR-17-FG-015963-01
Fagron	Tanino	16D08-B04-328410	23501	40	20160425

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Tanino*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 5 reference samples from the substance/substance group *Tanino*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tanino	16074504	23205	40
Fagron	Tanino	20F16-B04-203751	25751	50
Fagron	Tanino	21C15-B08-210552	25902	40
Caelo	Tanino	22001643	26254SI†	20
Fagron	Tanino	21C15-B08-210552	25902SI	40

- 201 894 spectra from a total of 4041 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 618 spectra from 373 *Apo-Ident* customers from 160 batches from the substance/substance group *Tanino*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 153 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tanino	20F16-B04-203751	1
	Tanino	21C15-B08-210552	2
	Tanino	22001643003	2
	Tanino	22001643011	4
A.H.D.	Tanino	13E27-N08	1
AHC	Tanino	20004500007	1
ALH	Tanino	14031919	1
ALH	Tanino	15091515	1
Alliance Healthcare	Tanino	12336001	1
Alliance	Tanino	200004500002	1
Caelo	Tanino		1
Caelo	Tanino	10019007	1
Caelo	Tanino	10315107	2
Caelo	Tanino	10315110	2
Caelo	Tanino	1091503	1
Caelo	Tanino	11302307	5
Caelo	Tanino	12171101	4
Caelo	Tanino	12171103	2
Caelo	Tanino	12171106	7
Caelo	Tanino	1217112263904	1
Caelo	Tanino	12336001	11
Caelo	Tanino	12336005	2
Caelo	Tanino	12336007	2
Caelo	Tanino	12336009	10
Caelo	Tanino	12336011	1
Caelo	Tanino	12336013	5
Caelo	Tanino	12336014	5
Caelo	Tanino	12336016	7
Caelo	Tanino	1236001	1
Caelo	Tanino	12A27-N01	1
Caelo	Tanino	13031401	1
Caelo	Tanino	14031901	2
Caelo	Tanino	14031903	5
Caelo	Tanino	14031905	3
Caelo	Tanino	14031912	4
Caelo	Tanino	14031913	2
Caelo	Tanino	14031915	2
Caelo	Tanino	14031918	4
Caelo	Tanino	14031919	6
Caelo	Tanino	14031920	2
Caelo	Tanino	15091503	3
Caelo	Tanino	15091504	4
Caelo	Tanino	15091506	1
Caelo	Tanino	15091509	18
Caelo	Tanino	15091511	2
Caelo	Tanino	15091512	1
Caelo	Tanino	15091515	15
Caelo	Tanino	1509509	1
Caelo	Tanino	1524308	1
Caelo	Tanino	15243801	11
Caelo	Tanino	15243802	3
Caelo	Tanino	15F23-B01-326357	1
Caelo	Tanino	16074504	15
Caelo	Tanino	16074505	1
Caelo	Tanino	16074507	1
Caelo	Tanino	16074509	8
Caelo	Tanino	16074509/171027T	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tanino	16074516	13
Caelo	Tanino	16074517	1
Caelo	Tanino	16074518	8
Caelo	Tanino	16D08-B04-328410	1
Caelo	Tanino	16D08-B04-334834	1
Caelo	Tanino	16D08-B04-354470	1
Caelo	Tanino	17343502	1
Caelo	Tanino	17343503	1
Caelo	Tanino	17343504	13
Caelo	Tanino	17343505	1
Caelo	Tanino	17343509	8
Caelo	Tanino	17343511	2
Caelo	Tanino	17343515	13
Caelo	Tanino	17343518	1
Caelo	Tanino	17343519	1
Caelo	Tanino	17343520	12
Caelo	Tanino	1734515	1
Caelo	Tanino	18017701	6
Caelo	Tanino	191382001	1
Caelo	Tanino	191382002	2
Caelo	Tanino	191382003	1
Caelo	Tanino	191382006	19
Caelo	Tanino	191382007	2
Caelo	Tanino	19138202	5
Caelo	Tanino	19138203	16
Caelo	Tanino	19138204	1
Caelo	Tanino	20002512002	23
Caelo	Tanino	20004500002	17
Caelo	Tanino	20004500007	7
Caelo	Tanino	20004500011	3
Caelo	Tanino	20045000007	1
Caelo	Tanino	21101305	1
Caelo	Tanino	22001643003	4
Caelo	Tanino	22001643011	1
Caelo	Tanino	2211Q-01052	1
Caelo	Tanino	28011502	1
Caelo	Tanino	318E-01052	1
Caelo	Tanino	320E01052	1
Caelo	Tanino	3513A-01052	1
Caelo	Tanino	41161-01052	1
Caelo	Tanino	4413I1052	1
Caelo	Tanino	70132238	1
Caelo	Tanino	9128607	2
Caelo	Tanino	9128608	1
Caelo	Tanino	91382031	1
Caelo	Tanino	B01-326357	1
Caelo	Tanino	B04-1976109	1
Caelo	Tanino	B04-2037501	1
Caelo	Tanino	Tannin20004500002	1
Caeol/ Noweda	Tanino	16074505	1
Caesar & Loretz GmbH...	Tanino	19138203	1
Caesar & Loretz GmbH...	Tanino	191382006	1
Caesar & Loretz GmbH...	Tanino	20004500002	1
Caesar & Loretz GmbH...	Tanino	191382006	1
Caesar & Loretz GmbH...	Tanino	20004500003	1
Caesar & Loretz GmbH...	Tanino	20004500002	1
Caesar & Loretz GmbH...	Tanino	191382006	1
Caesar & Loretz GmbH...	Tanino	17343520	1
Caesar & Loretz GmbH...	Tanino	20002512002	1
Caesar & Loretz GmbH...	Tanino	20002512003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH…	Tanino	20004500002	1
Caesar & Loretz GmbH/Otto	Tanino	20002512002	1
Caesar & Loretz GmbH…	Tanino	20004500002	1
Caesar & Loretz GmbH…	Tanino	20004500002	1
Caesar & Loretz GmbH…	Tanino	200004500001	1
Caesar & Loretz GmbH…	Tanino	20004500002	1
Caesar & Loretz GmbH	Tanino	16D08-B04	1
Caesar & Loretz GmbH	Tanino	17343509	1
Caesar & Loretz GmbH	Tanino	17343515	2
Caesar & Loretz GmbH	Tanino	17343520	6
Caesar & Loretz GmbH	Tanino	191382006	5
Caesar & Loretz GmbH	Tanino	191382007	1
Caesar & Loretz GmbH	Tanino	19138202	1
Caesar & Loretz GmbH	Tanino	19138203	3
Caesar & Loretz GmbH	Tanino	20002512001	1
Caesar & Loretz GmbH	Tanino	20002512002	5
Caesar & Loretz GmbH	Tanino	20004500002	10
Caesar & Loretz GmbH	Tanino	20F16-B04-197619	1
Caesar & Loretz	Tanino	16074504	1
Caesar Loretz	Tanino	20002512002	1
Caesar/Lorenz	Tanino	11302307	1
Caleo/Phoenix	Tanino	14K17-B08-306993	1
Ebert u. Jacobi 1…	Tanino	15091509	1
Euro OTC	Tanino	15091509	1
Euro OTC	Tanino	16074501	1
Euro OTC	Tanino	16074509	1
Euro OTC	Tanino	18017701	1
Euro OTC	Tanino	4117I-01052	1
Fagron	Tanino	1014A-01052	1
Fagron	Tanino	11C09-N05	1
Fagron	Tanino	12A27-N01	1
Fagron	Tanino	12E21-N04	4
Fagron	Tanino	12H14N05	1
Fagron	Tanino	12H14-N05	5
Fagron	Tanino	13B28-N08	1
Fagron	Tanino	13E27-N08	1
Fagron	Tanino	13H30-B03287645	1
Fagron	Tanino	13H30-B03-287645	2
Fagron	Tanino	14A07-B01-293468	5
Fagron	Tanino	14e07-b03-298480	1
Fagron	Tanino	14E07-B03-298480	2
Fagron	Tanino	14J06-B04	1
Fagron	Tanino	14J06-B04-0858	1
Fagron	Tanino	14J06B04299398	2
Fagron	Tanino	14J06-B04-299398	2
Fagron	Tanino	14K17-B08-306993	1
Fagron	Tanino	15F23-B01	1
Fagron	Tanino	15F23-B01-322984	3
Fagron	Tanino	15F23B01326357	1
Fagron	Tanino	15F23-B01-326357	1
Fagron	Tanino	160300029	1
Fagron	Tanino	160300126	1
Fagron	Tanino	160300146	2
Fagron	Tanino	1603001788	1
Fagron	Tanino	160300178B	3
Fagron	Tanino	163001788	1
Fagron	Tanino	16D08-b04	1
Fagron	Tanino	16D08B04	2
Fagron	Tanino	16D08-B04	2
Fagron	Tanino	16D08-B04-328410	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tanino	16D08-B04-334834	3
Fagron	Tanino	16D08B04335787	1
Fagron	Tanino	16D08-B04-335787	2
Fagron	Tanino	16D08-B04-337161	1
Fagron	Tanino	16D08-B04-352128	3
Fagron	Tanino	16D08-B04-354470	3
Fagron	Tanino	16D08B04354470	1
Fagron	Tanino	20F16-B04	1
Fagron	Tanino	20F16-B04-197619	8
Fagron	Tanino	20F16-B04-2033751	2
Fagron	Tanino	20F16-B04-203751	10
Fagron	Tanino	20F16-bo4-203751	1
Fagron	Tanino	21C15-B08	1
Fagron	Tanino	21C15-B08-210552	5
Fagron	Tanino	21C5-B08-210552	1
Fagron	Tanino	2212M-01052	1
Fagron	Tanino	2DF16-B04-203751	1
Fagron	Tanino	3518M-01052	1
Fagron	Tanino	4-20375001	1
Fagron	Tanino	B04-2037501	2
Fiebig	Tanino	16074518	1
Frago/Gehe	Tanino	15F23-B01	1
Gatt-Koller / Phoenix	Tanino	3335/08134613	1
Gatt-Koller / Phoenix	Tanino	333508134613	2
Gehe	Tanino	12171106	1
Gehe	Tanino	12336016	2
Gehe	Tanino	12H14-N05	1
Gehe	Tanino	15091506	1
Gehe	Tanino	16074504	1
Gehe	Tanino	20002512002	1
Gehe	Tanino	20004500002	1
Gehe	Tanino	21C15-B08-210552	1
Hirsch	Tanino	1811209	1
INTERN-DROGEN	Tanino	20004500002	1
Kehr	Tanino	22001643011	1
L10	Tanino	17343509	1
Nachprüfung	Tanino	5210A-01052	1
Noweda	Tanino	16074509	1
Noweda	Tanino	17343520	1
Noweda	Tanino	191382006	1
Phoenix	Tanino	12336013	1
Phoenix	Tanino	16074509	1
Phönix	Tanino	10313107Retest	1
Phönix	Tanino	10315110	1
phönix	Tanino	14E07-B03-293744	1
phönix	Tanino	15/AKD65	1
Phönix	Tanino	17343520	1
Sanacorp WE: 26.01.1…	Tanino	14031912	1
Sanacorp	Tanino		1
Sanacorp	Tanino	12171102	1
Sanacorp	Tanino	12336011	1
Sanacorp	Tanino	12336014	1
Sanacorp	Tanino	14031912	1
Sanacorp	Tanino	16D08-B04	1
Sanacorp	Tanino	21C15-B08-210552	1
Sanacorp	Tanino	22001613011	2
Sanacorp	Tanino	22001643003	1
Synopharm/Anzag	Tanino	3411I-01052	1

- 235 449 spectra from 1515 *Apo-Ident* customers from a total of 49 100 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tanino* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tanino* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	190	0	201 894
Type C	0	602	16	235 449

The substance/substance group *Tanino* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	97.4110 % (> 96.9256 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21608	23211	46,90	126,76
21653	21653	0,00	119,38
23211	23211	0,00	131,90
23501	23211	8,96	128,99
23631	23631	0,00	111,66
25516	23211	21,95	134,19
26254	26254	0,00	116,12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tartarato de L-Carnitina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21107-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tartarato de L-Carnitina; L-Carnitina Tartarato; Levocarnitina Tartarato; Tartarato de L-carnitina; Tartarato de Levocarnitina

Special notes

When selecting the *Tartarato de L-Carnitina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tartarato de L-Carnitina	4	7	0

Second-stage model

For differentiation of the substance/substance group *Tartarato de L-Carnitina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tartarato de L-Carnitina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	112,91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tartarato de L-Carnitina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tartarato de L-Carnitina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tartarato de L-carnitina	10100220240309	BR20018	40	20260228*
Dr. Behr	Tartarato de L-Carnitina	WE11060069	21107	40	from supplier
Dr. Behr	Tartarato de L-Carnitina	WE15080050	22265	60	from supplier
Euro OTC	Tartarato de L-Carnitina	1302017-01	21206	40	from supplier

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Tartarato de L-Carnitina*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 782 spectra from a total of 2838 batches from further 484 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 8 reference samples from the substance/substance group *Tartarato de L-Carnitina*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tartarato de L-Carnitina	1708023	23697	40
Euro OTC	Tartarato de L-Carnitina	2007043	25395	40
Euro OTC	Tartarato de L-Carnitina	2105018	25712	50
Euro OTC	Tartarato de L-Carnitina	2207004	26422	40
Euro OTC	Tartarato de L-Carnitina	2305008	26865	40
Pharmorgana	Tartarato de L-Carnitina	1000160672	22957	40
Pharmorgana	Tartarato de L-Carnitina	1000170113	24108	40
Fagron	Tartarato de L-carnitina	10100220240309	BR20018SI†	20

- 201 774 spectra from a total of 4037 batches from further 841 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Tartarato de L-Carnitina*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Tartarato de L-Carnitina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tartarato de L-Carnitina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	310	0	201 774
Type C	0	0	0	236 067

The substance/substance group *Tartarato de L-Carnitina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21107	21107	0,00	224,60
21206	21206	0,00	222,40
22265	22265	0,00	227,09
BR20018	BR20018	0,00	213,44

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tartarato de metoprolol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21753-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tartarato de metoprolol; Metoprolol, tartarato; Metoprololi tartras

Special notes

When selecting the *Tartarato de metoprolol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tartarato de metoprolol	7	3	75

Second-stage model

For differentiation of the substance/substance group *Tartarato de metoprolol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tartarato de metoprolol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	111,72	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tartarato de metoprolol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tartarato de metoprolol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Tartarato de metoprolol	APMTP02218MT	24596	40	20190220
Euro OTC	Tartarato de metoprolol	2001021	25098	40	20200116*
Euro OTC	Tartarato de metoprolol	2211008	26429	40	20221215*
Euro OTC	Tartarato de metoprolol	2211008	26429SI	20	20221215*
Fagron	Tartarato de metoprolol	16E31-B03-327107	22927	40	20160627
Fagron	Tartarato de metoprolol	16E31-B03-327107	22943	40	20160627
Fagron	Tartarato de metoprolol	16E31-B03-327107	22944	40	20160627
Fagron	Tartarato de metoprolol	19K20-F03-366934	25061	40	20191218
Inresa	Tartarato de metoprolol	309905RII	21753	60	AR-15-FG-006635-01
Inresa	Tartarato de metoprolol	405005RII	21805	60	20140430

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Tartarato de metoprolol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 542 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Tartarato de metoprolol*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tartarato de metoprolol	18K26-B01-359370	24825	40
Fagron	Tartarato de metoprolol	21E10-F03-378925	25752	40
Inresa	Tartarato de metoprolol	405005RIIC	22908	40

- 201 964 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 296 spectra from 192 *Apo-Ident* customers from 82 batches from the substance/substance group *Tartarato de metoprolol*.

- Among them are spectra of independent samples from 75 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tartarato de metoprolol		1
	Tartarato de metoprolol	2001021-02	4
	Tartarato de metoprolol	210530SRII	1
	Tartarato de metoprolol	2211008-01	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Tartarato de metoprolol	22F02-B19-220195	3
AHD	Tartarato de metoprolol	22F02-B19-220195	2
Andor	Tartarato de metoprolol	APMTP0117MT	1
Antares	Tartarato de metoprolol	1014Q-07308	1
apomix	Tartarato de metoprolol	18K26-B01-355911	1
Audor Pharma	Tartarato de metoprolol	APMTP00117MT	17
Audor Pharma	Tartarato de metoprolol	APMTP02218	1
Audor Pharma	Tartarato de metoprolol	APMtP02218Mt	1
Audor Pharma	Tartarato de metoprolol	APMTP02218MT	16
Audor Pharma	Tartarato de metoprolol	APMTPOC117MT	1
Audor Pharma	Tartarato de metoprolol	MTP00117MT	1
Audor Pharma	Tartarato de metoprolol	MTP02218	1
Caelo	Tartarato de metoprolol	1729314P-200715-1	1
Caelo	Tartarato de metoprolol	17G03-B09-351672	1
Caelo	Tartarato de metoprolol	1919I-03763	1
Caelo	Tartarato de metoprolol	APMT00117MT	1
EuRho	Tartarato de metoprolol	2001021-02	2
Euro OTC	Tartarato de metoprolol	2001021	1
Euro OTC	Tartarato de metoprolol	200102101	1
Euro OTC	Tartarato de metoprolol	2001021-01	61
Euro OTC	Tartarato de metoprolol	2001021-02	8
Euro OTC	Tartarato de metoprolol	201021-01	1
Euro OTC	Tartarato de metoprolol	AP20112701	1
Euro OTC	Tartarato de metoprolol	Meto08122022	1
Euro OTC	Tartarato de metoprolol	MTP02218	3
Fagro	Tartarato de metoprolol	16MD000095	1
Fagron	Tartarato de metoprolol	16E31-B03-325535	1
Fagron	Tartarato de metoprolol	16E31-B03-327107	23
Fagron	Tartarato de metoprolol	1700305RII	1
Fagron	Tartarato de metoprolol	17G03-B03-353935	1
Fagron	Tartarato de metoprolol	17G03-B09	1
Fagron	Tartarato de metoprolol	17G03-B09-340197	3
Fagron	Tartarato de metoprolol	17G03-B09-342813	2
Fagron	Tartarato de metoprolol	17G03-B09-345302	1
Fagron	Tartarato de metoprolol	17G03-B09-347089	1
Fagron	Tartarato de metoprolol	17G03-B09-347304	1
Fagron	Tartarato de metoprolol	17g03-B09-350669	1
Fagron	Tartarato de metoprolol	17G03-B09-350669	4
Fagron	Tartarato de metoprolol	17G03-B09-351672	1
Fagron	Tartarato de metoprolol	17G03-B09-353935	2
Fagron	Tartarato de metoprolol	1802705RII	1
Fagron	Tartarato de metoprolol	18K26-B01	2
Fagron	Tartarato de metoprolol	18K26-B01-355910	1
Fagron	Tartarato de metoprolol	18K26-B01-355911	2
Fagron	Tartarato de metoprolol	18K26-B01-359370	7
Fagron	Tartarato de metoprolol	18K26-B01-359371	7
Fagron	Tartarato de metoprolol	18K26-B01-362451	3
Fagron	Tartarato de metoprolol	18KS26-B01	1
Fagron	Tartarato de metoprolol	1902205RII	1
Fagron	Tartarato de metoprolol	1902205RII	1
Fagron	Tartarato de metoprolol	190205RII	1
Fagron	Tartarato de metoprolol	19K20-F03	1
Fagron	Tartarato de metoprolol	19K20-F03-366934	7
Fagron	Tartarato de metoprolol	19K20-F03-366935	1
Fagron	Tartarato de metoprolol	19K20-F03-366936	1
Fagron	Tartarato de metoprolol	20H06-F04	2
Fagron	Tartarato de metoprolol	20H06F04373426	3
Fagron	Tartarato de metoprolol	20H06-F04-373426	4
Fagron	Tartarato de metoprolol	2100605RII	1
Fagron	Tartarato de metoprolol	21E-10-F03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tartarato de metoprolol	21E10-F03-378925	12
Fagron	Tartarato de metoprolol	21E10-F03-378925/2100605RII	1
Fagron	Tartarato de metoprolol	21E10-F03378926	1
Fagron	Tartarato de metoprolol	21E10-F03-378926	3
Fagron	Tartarato de metoprolol	21E10-F03-78926	1
Fagron	Tartarato de metoprolol	22F02-B19-220195	1
Fagron	Tartarato de metoprolol	22F02-B19-220257	1
Fagron	Tartarato de metoprolol	B01-3593700	1
Fagron	Tartarato de metoprolol	B01-3624501	1
Fagron	Tartarato de metoprolol	F03-3669304	2
Fagron	Tartarato de metoprolol	F03-3789205	4
Fagron	Tartarato de metoprolol	F04-3734206	1
Fagron	Tartarato de metoprolol	F03-3789205	1
Gehe	Tartarato de metoprolol	21E-10-F03	1
Gehe	Tartarato de metoprolol	2211008-01	3
Gehe	Tartarato de metoprolol	22F02-B19-220195	1
HELIOS Klinikum Erfu…	Tartarato de metoprolol	405005RIIC	1
Inresa	Tartarato de metoprolol	4050005RIIB	1
Inresa	Tartarato de metoprolol	405005RIIB	1
Inresa	Tartarato de metoprolol	504005RIIC/29082016	1
Jenne	Tartarato de metoprolol	2211008-01	1
Klosterring	Tartarato de metoprolol	17G03-B09-345301	1
Noweda 21.06.22 EK 34,95	Tartarato de metoprolol	2001021-01	1
Noweda	Tartarato de metoprolol	18K26-B01-3593705	1
Noweda	Tartarato de metoprolol	18K26-B01-362451	1
Noweda	Tartarato de metoprolol	21E10-F03	1
Noweda	Tartarato de metoprolol	2211008-01	1
Noweda	Tartarato de metoprolol	22F02-B19-220195	1
Noweda	Tartarato de metoprolol	F03-3789206	1
Phönix	Tartarato de metoprolol	21E10-F03	1
Sanacorp	Tartarato de metoprolol	2001021-01	3
Sanacorp	Tartarato de metoprolol	2211008-01	3
Sidonia	Tartarato de metoprolol	405005RIIC/09062017	1
Sigma Adrich/Alliance H.	Tartarato de metoprolol	PHR1076	1
Sigma-Aldrich GmbH	Tartarato de metoprolol	LRAA6905	4
Th. Geyer	Tartarato de metoprolol	56392-17-7	1

- 235 771 spectra from 1515 *Apo-Ident* customers from a total of 49 177 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tartarato de metoprolol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tartarato de metoprolol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	120	0	201 964
Type C	0	291	5	235 771

The substance/substance group *Tartarato de metoprolol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.3108 % (> 97.2973 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21753	21753	0,00	146,15
21805	21753	5,30	146,75
22927	21753	9,26	141,98
22943	21753	4,68	144,75
22944	25098	7,12	140,54
24596	25098	8,18	141,59
25061	21753	9,40	147,67
25098	25098	0,00	140,54
26429	26429	0,00	142,21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Taurina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20403-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Taurina

Special notes

When selecting the *Taurina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Taurina	9	5	14

Second-stage model

For differentiation of the substance/substance group *Taurina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Taurina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	125,73	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Taurina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Taurina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Taurina	1306024-01	21108	50	20130822
Euro OTC	Taurina	1504032-01	21893	60	20150430
Euro OTC	Taurina	1504032-01	21992	60	9167
Euro OTC	Taurina	1602011	22370	60	20160218*
Euro OTC	Taurina	1607035	22795	40	20160819*
Euro OTC	Taurina	1704001	23177	40	20170426*
Euro OTC	Taurina	1904003	24632	40	20190425*
Euro OTC	Taurina	2004002	25406	40	20200615*
Euro OTC	Taurina	2206003	26222	40	20220629*
Euro OTC	Taurina	2206003	26222SI	20	20220629*
Euro OTC	Taurina	2301048	26749	40	20230511*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 490 spectra of 11 reference samples from the substance/substance group *Taurina*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 472 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Taurina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Taurina	1711006	23739	40
Euro OTC	Taurina	1810006	24310	40
Euro OTC	Taurina	1910017	24977	40
Euro OTC	Taurina	2309005	26927	40
Euro OTC	Taurina	2310009	26991	40
Euro OTC	Taurina	2301048	26749SI†	20
Euro OTC	Taurina	2309005	26927SI	20

- 201 844 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 31 spectra from 10 *Apo-Ident* customers from 14 batches from the substance/substance group *Taurina*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caelo	Taurina	1704001-01	2
el compra import	Taurina	1609025	1
elcompra	Taurina	xp17013244	1
Euro OTC	Taurina	1704001-01	1
Euro OTC	Taurina	1904003-01	1
Euro OTC	Taurina	1910017-01	1
Euro OTC	Taurina	2004002-01	7
Euro OTC	Taurina	2008013-01	6
Euro OTC	Taurina	2008013-02	2
Euro OTC	Taurina	2008013-03	1
Euro OTC	Taurina	2206003-01	4
Euro OTC	Taurina	2301048-01	1
Euro OTC	Taurina	XP16023196	1
Gall Pharma / Phoenix	Taurina		1
hannes	Taurina	1202125	1

- 236 036 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Taurina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Taurina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	490	0	152 472
Type B	0	240	0	201 844
Type C	0	31	0	236 036

The substance/substance group *Taurina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7755 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 80.6452 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21108	22370	4,14	121,69
21893	22370	3,89	121,09
21992	21992	0,00	121,56
22370	22370	0,00	120,93
22795	22795	0,00	121,56
23177	23177	0,00	120,81
24632	24632	0,00	121,17
25406	25406	0,00	122,23
26222	26222	0,00	121,23
26749	26749	0,00	121,83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Teofilina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20723-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Teofilina; Theophyllinum

Special notes

When selecting the *Teofilina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Teofilina	6	3	13

Second-stage model

For differentiation of the substance/substance group *Teofilina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Teofilina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de midazolam	112,26	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Teofilina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Teofilina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Teofilina	12166316	20723	40	1402055
Caelo	Teofilina	12341101	21740	60	20121115
Caelo	Teofilina	192563	24902	40	20191120*
Caelo	Teofilina	22001229002	26236	40	20220505
Caelo	Teofilina	24001902	27317	40	20240819*
Gatt-Koller	Teofilina	23J01412	27095	30	20230809

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 250 spectra of 6 reference samples from the substance/substance group *Teofilina*. These samples

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 712 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Teofilina*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Teofilina	15203018	23253	40
Caelo	Teofilina	171962	23854	40
Caelo	Teofilina	23001176	26838	40
Caelo	Teofilina	22001229002	26236SI†	20
Caelo	Teofilina	23001176	26838SI	20
Gatt-Koller	Teofilina	23J01412	27095SI†	20

- 201 904 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 21 *Apo-Ident* customers from 15 batches from the substance/substance group *Teofilina*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Teofilina	22001229009	1
Alliance Healthcare	Teofilina	192563003	1
Caelo	Teofilina	12166305	2
Caelo	Teofilina	12166306	1
Caelo	Teofilina	12166311	1
Caelo	Teofilina	12166312	3
Caelo	Teofilina	12166315	1
Caelo	Teofilina	12341101	2
Caelo	Teofilina	12341104	1
Caelo	Teofilina	15203010	1
Caelo	Teofilina	17196203	2
Caelo	Teofilina	18097508	1
Caelo	Teofilina	22001229002	1
Caelo	Teofilina	22001229006	1
Caesar & Loretz GmbH	Teofilina	21000106001	1
Caesar & Loretz GmbH	Teofilina	22001229002	1
Caesar&loretz,Phoenix	Teofilina	12166315	1
Caeser und Loretz GmbH	Teofilina	18097508	1
Noweda	Teofilina	12166305	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 243 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Teofilina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Teofilina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	250	0	152 712
Type B	0	180	0	201 904
Type C	0	24	0	236 043

The substance/substance group *Teofilina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 75.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20723	20723	0,00	254,97
21740	20723	16,47	269,15
24902	24902	0,00	253,95
26236	24902	7,77	253,10
27095	20723	13,45	243,80
27317	27317	0,00	248,08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Teofilina etilenodiamina hidratada**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20831-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Teofilina etilenodiamina hidratada; Theophyllinum et ethylendiaminum hydricum

Special notes

When selecting the *Teofilina etilenodiamina hidratada* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Teofilina etilenodiamina hidratada	7	5	2

Second-stage model

For differentiation of the substance/substance group *Teofilina etilenodiamina hidratada* the following second-stage model is used:

- Submodelo 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Teofilina etilenodiamina hidratada* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glicina	106,12	–
⋮	⋮	⋮
Clioquinol	>50	20,49
Mesalazina	>50	46,19
Nitrato de miconazol	>50	49,72
Ácido nicotínico	>50	112,58

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Teofilina etilenodiamina hidratada* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Teofilina etilenodiamina hidratada*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Teofilina etilenodiamina ...	12145301	20831	40	20120628
Caelo	Teofilina etilenodiamina ...	12363708	20992	40	20130116
Caelo	Teofilina etilenodiamina ...	13268609	21549	40	1412133
Caelo	Teofilina etilenodiamina ...	15380302	22589	40	20160211
Caelo	Teofilina etilenodiamina ...	17073707	23564	30	20170323
Caelo	Teofilina etilenodiamina ...	192220	24903	40	20191204*
Caelo	Teofilina etilenodiamina ...	20004052	25510	40	20201201

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Teofilina etilenodiamina hidratada*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 692 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 8 reference samples from the substance/substance group *Teofilina etilenodiamina hidratada*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Teofilina etilenodiamina …	172999	23823	40
Caelo	Teofilina etilenodiamina …	182738	24383	40
Caelo	Teofilina etilenodiamina …	22000118006	25974	40
Caelo	Teofilina etilenodiamina …	22003464	26499	40
Caelo	Teofilina etilenodiamina …	23003143	27237	40
Caelo	Teofilina etilenodiamina …	22000118006	25974SI	10
Caelo	Teofilina etilenodiamina …	22003464	26499SI	20
Caelo	Teofilina etilenodiamina …	23003143	27237SI	20

- 201 834 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Teofilina etilenodiamina hidratada*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
ACM / Phoenix	Teofilina etilenodiamina ...	KNC0896J14	1
Caelo	Teofilina etilenodiamina ...	15380302	1
Caelo	Teofilina etilenodiamina ...	20003320003	1
Caesar & Loretz GmbH	Teofilina etilenodiamina ...	20003320003	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Teofilina etilenodiamina hidratada* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Teofilina etilenodiamina hidratada* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	250	0	201 834
Type C	0	4	0	236 063

The substance/substance group *Teofilina etilenodiamina hidratada* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20831	21549	9,61	153,64
20992	21549	5,56	152,40
21549	21549	0,00	150,97
22589	24903	7,59	157,99
23564	24903	9,72	161,06
24903	24903	0,00	156,83
25510	21549	14,40	158,76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Testosterona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20961-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Testosterona; Testosteronum

Special notes

When selecting the *Testosterona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Testosterona	14	20	114

Second-stage model

For differentiation of the substance/substance group *Testosterona* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Testosterona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prasterona	68,82	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Testosterona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Testosterona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Testosterona	13406004	21370	50	20131219
Caelo	Testosterona	13406004	21371	50	20131219
Caelo	Testosterona	15244906	21987	60	20150814
Caelo	Testosterona	15244906	21987SI	38	20150814
Caelo	Testosterona	16311506	23244	40	20161123
Euro OTC	Testosterona	1307001-01	20961	40	1402309
Euro OTC	Testosterona	1511005	22232	60	20151119*
Euro OTC	Testosterona	1511005	22232SI	35	20151119*
Euro OTC	Testosterona	1604049	22561	40	20160510*
Euro OTC	Testosterona	1604049	22561SI	34	20160510*
Euro OTC	Testosterona	1910001	24963	40	20191024*
Euro OTC	Testosterona	1912017	25104	40	20191216*
Euro OTC	Testosterona	2005006	25160	40	20200519*
Euro OTC	Testosterona	2005006	25160SI	27	20200519*
Euro OTC	Testosterona	2403002	27212	40	20240502*
Fagron	Testosterona	12F13-N02	20729	40	20120628
Fagron	Testosterona	15E18-B08-307772	21970	60	20150526
Fagron	Testosterona	15E18-B08-307772	21970SI	54	20150526
Fagron	Testosterona	17J26-B01-342032	23764	40	20171205
Fagron	Testosterona	22H08-B02-222389	26392	40	20220905
Fagron	Testosterona	22H08-B02-222389	26392SI	40	20220905

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 908 spectra of 21 reference samples from the substance/substance group *Testosterona*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.
- 152 054 spectra from a total of 2828 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1815 spectra of 47 reference samples from the substance/substance group *Testosterona*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Testosterona	171199	23347	40
Caelo	Testosterona	181478	24265	40
Caelo	Testosterona	191113	24520	40
Caelo	Testosterona	21002048	25794	40
Euro OTC	Testosterona	1511005-01	21994	60
Euro OTC	Testosterona	1607013	22707	40
Euro OTC	Testosterona	1702017	23146	40
Euro OTC	Testosterona	1802015	23948	40
Euro OTC	Testosterona	1805006	24131	40
Euro OTC	Testosterona	1805021	24132	40
Euro OTC	Testosterona	1808033	24201	40
Euro OTC	Testosterona	1811027	24422	40
Euro OTC	Testosterona	1912014	24964	40
Euro OTC	Testosterona	2008038	25308	40
Euro OTC	Testosterona	2008032	25327	40
Euro OTC	Testosterona	2106009	25705	50
Euro OTC	Testosterona	2110010	25877	50

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Testosterona	2206013	26215	40
Euro OTC	Testosterona	2311029	27004	40
Euro OTC	Testosterona	2407002	27341	40
Caelo	Testosterona	16311506	23244SI†	30
Caelo	Testosterona	171199	23347SI	28
Caelo	Testosterona	171199	23670	40
Caelo	Testosterona	171199	23670SI	30
Caelo	Testosterona	181478	24265SI	40
Caelo	Testosterona	191113	24520SI	40
Caelo	Testosterona	21002048	25794SI	40
Euro OTC	Testosterona	1511005-01	21994SI	32
Euro OTC	Testosterona	1607013	22707SI	40
Euro OTC	Testosterona	1702017	23146SI	21
Euro OTC	Testosterona	1802015	23948SI	40
Euro OTC	Testosterona	1805006	24131SI	40
Euro OTC	Testosterona	1805021	24132SI	40
Euro OTC	Testosterona	1808033	24201SI	40
Euro OTC	Testosterona	1811027	24422SI	26
Euro OTC	Testosterona	1910001	24963SI†	39
Euro OTC	Testosterona	1912014	24964SI	30
Euro OTC	Testosterona	1912017	25104SI†	40
Euro OTC	Testosterona	2008038	25308SI	36
Euro OTC	Testosterona	2008032	25327SI	40
Euro OTC	Testosterona	2106009	25705SI	49
Euro OTC	Testosterona	2110010	25877SI	50
Euro OTC	Testosterona	2206013	26215SI	40
Euro OTC	Testosterona	2311029	27004SI	32
Euro OTC	Testosterona	2403002	27212SI†	30
Euro OTC	Testosterona	2407002	27341SI	32
Fagron	Testosterona	17J26-B01-342032	23764SI†	30

- 200 269 spectra from a total of 4020 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 369 spectra from 111 *Apo-Ident* customers from 122 batches from the substance/substance group *Testosterona*.

- Among them are spectra of independent samples from 114 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Testosterona	2206013-02	4
	Testosterona	23000429008	1
	Testosterona	2311029-01	1
	Testosterona	23K14-B10230723	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Testosterona	23K14-B10-230723	1
	Testosterona	2403002	1
Audor Pharma	Testosterona	AP5106061T	5
Audor Pharma	Testosterona	APZTST16001-M1T	1
Audor Pharma	Testosterona	APZTSTG18003T	10
Audor Pharma	Testosterona	apztstg18004t	2
Audor Pharma	Testosterona	APZTSTG18004T	3
Caelo	Testosterona		1
Caelo	Testosterona	11/07-N12	1
Caelo	Testosterona	12176301	1
Caelo	Testosterona	12176305	3
Caelo	Testosterona	13134804	1
Caelo	Testosterona	13134806	4
Caelo	Testosterona	13134808	1
Caelo	Testosterona	13406004	2
Caelo	Testosterona	14201105	1
Caelo	Testosterona	14355605	1
Caelo	Testosterona	15195802	1
Caelo	Testosterona	15195803	1
Caelo	Testosterona	15244906	1
Caelo	Testosterona	15412201	5
Caelo	Testosterona	15412202	3
Caelo	Testosterona	1604049-01	1
Caelo	Testosterona	16225804	3
Caelo	Testosterona	16225807	2
Caelo	Testosterona	16311506	1
Caelo	Testosterona	17119902	2
Caelo	Testosterona	17119903	1
Caelo	Testosterona	17119911	1
Caelo	Testosterona	1805021-01	2
Caelo	Testosterona	1811027-01	1
Caelo	Testosterona	18147803	7
Caelo	Testosterona	18147810	1
Caelo	Testosterona	19111302	1
Caelo	Testosterona	192738003	1
Caelo	Testosterona	192738006	5
Caelo	Testosterona	192738009	1
Caelo	Testosterona	19273803	2
Caelo	Testosterona	20004205001	1
Caelo	Testosterona	20004205002	1
Caelo	Testosterona	20004205004	1
Caelo	Testosterona	21002048002	2
Caelo	Testosterona	21002048003	1
Caelo	Testosterona	21002048004	2
Caelo	Testosterona	21002048009	7
Caelo	Testosterona	21002048010	1
Caelo	Testosterona	AP5106061T	1
Caelo	Testosterona	APL00034466T	1
Caelo	Testosterona	APZTSTG18004T	1
Caesar & Loretz GmbH...	Testosterona	21002048002	1
Caesar & Loretz GmbH	Testosterona	18147803	1
Caesar & Loretz GmbH	Testosterona	19273804	2
Caesar & Loretz GmbH	Testosterona	20004205002	1
Caesar & Loretz GmbH	Testosterona	20004205007	1
Caesar & Loretz GmbH	Testosterona	21002048002	1
erou	Testosterona	2110010-02	1
EuRho	Testosterona	1811027	1
Euro OTC	Testosterona	1106011-01	1
Euro OTC	Testosterona	1106011-03	4
Euro OTC	Testosterona	11o6011-03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Testosterona	1207005-02	1
Euro OTC	Testosterona	130700101	1
Euro OTC	Testosterona	1307001-01	5
Euro OTC	Testosterona	140400201	1
Euro OTC	Testosterona	1404002-01	3
Euro OTC	Testosterona	1404002-1	1
Euro OTC	Testosterona	1511005-01	6
Euro OTC	Testosterona	1604049-01	17
Euro OTC	Testosterona	1607013-01	1
Euro OTC	Testosterona	1607013-02	9
Euro OTC	Testosterona	1702017-01	41
Euro OTC	Testosterona	1802015	1
Euro OTC	Testosterona	180500601	1
Euro OTC	Testosterona	1805006-01	1
Euro OTC	Testosterona	1805021-01	9
Euro OTC	Testosterona	180506-01	1
Euro OTC	Testosterona	1808033-01	3
Euro OTC	Testosterona	1811027	1
Euro OTC	Testosterona	1811027-01	10
Euro OTC	Testosterona	1811027-02	1
Euro OTC	Testosterona	18147813	2
Euro OTC	Testosterona	1910001-01	5
Euro OTC	Testosterona	1912014-01	5
Euro OTC	Testosterona	1912017-01	1
Euro OTC	Testosterona	2005006-01	2
Euro OTC	Testosterona	2008032-01	10
Euro OTC	Testosterona	2008038-01	14
Euro OTC	Testosterona	2008038-02	1
Euro OTC	Testosterona	2106009-01	9
Euro OTC	Testosterona	2106009-02	4
Euro OTC	Testosterona	2110010-01	7
Euro OTC	Testosterona	2110010-02	1
Euro OTC	Testosterona	2403002-01	1
Euro OTC	Testosterona	3x1106011-03	1
Euro OTC	Testosterona	APZTSTG18003T	1
Euro OTC	Testosterona	ZTSTy18004	1
Euro TOC	Testosterona	1811027-02	1
EUro/AHD	Testosterona	1106011-03	1
Euroo/Phoenix	Testosterona	1307001-01	1
Fagron	Testosterona	11/07-N12	1
Fagron	Testosterona	12F13-N02	1
Fagron	Testosterona	13g10n03	1
Fagron	Testosterona	13G10-N03	2
Fagron	Testosterona	13I26-N08	1
Fagron	Testosterona	13L09-B03-294148	1
Fagron	Testosterona	13l09b03294149	1
Fagron	Testosterona	13l09b03298118	1
Fagron	Testosterona	15E18-B08	1
Fagron	Testosterona	16A20-B11-318899	7
Fagron	Testosterona	1712-B05	1
Fagron	Testosterona	17A12-B05-331496	1
Fagron	Testosterona	17J26-B01-342033	2
Fagron	Testosterona	17J26-B01-342637	4
Fagron	Testosterona	18A25-B03-350800	2
Fagron	Testosterona	19B12-B01	5
Fagron	Testosterona	19J04-F04_365938	1
Fagron	Testosterona	19J04-F04-365936	1
Fagron	Testosterona	20804-F03-370229	3
Fagron	Testosterona	20B04-F03	1
Fagron	Testosterona	23K14-B10-233057	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Testosterona	24B26-B07-237509	1
Fagron	Testosterona	F03-3702209	1
Fagron	Testosterona	GTJ151103	1
Gatt-Koller	Testosterona	22J00592	1
Gehe	Testosterona	1805021-01	1
Gehe	Testosterona	1811027-01	3
GEHE	Testosterona	1912014-01	1
Geilenkirchen	Testosterona	16225803	1
Haihang Industry	Testosterona	20140114-1	1
Haihang Industry	Testosterona	20140114-2	1
Hubei Zhuxi Humanwell	Testosterona	2005006-01	1
Noweda	Testosterona	1702017-01	1
Noweda	Testosterona	19111303	1
Noweda	Testosterona	23000429008	1
Noweda	Testosterona	2311029-01	1
NWM CHina	Testosterona	TE150402	1
Pharbil Waltrop GmbH	Testosterona	9542100/228178-0	1
Phönix Gotha	Testosterona	1106011-03	1
Phönix Gotha	Testosterona	1408015-01	1
Sanacorp	Testosterona	2110010-01	1
Sanacorp	Testosterona	23000429006	1
Shandong Northwest M…	Testosterona	GTJ160510	1
Spirig	Testosterona	13406003	1

- 235 698 spectra from 1515 *Apo-Ident* customers from a total of 49 139 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Testosterona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Testosterona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	908	0	152 054
Type B	0	1815	0	200 269
Type C	0	363	6	235 698

The substance/substance group *Testosterona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3392 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6694 %)
Type C	100.0000 % (> 99.9007 %)	98.3740 % (> 97.5610 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20729	24963	14,17	132,21
20961	20961	0,00	133,50
21370	22232	7,73	132,27
21371	22232	8,86	132,66
21970	22232	4,10	132,32
21987	22232	3,35	133,14
22232	22232	0,00	133,44
22561	22561	0,00	125,49
23244	22232	6,22	133,39
23764	22232	6,35	133,95
24963	24963	0,00	132,78
25104	25104	0,00	136,17
25160	25160	0,00	131,72
26392	25104	15,02	134,91
27212	27212	0,00	135,19

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tetraborato de sódio**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20179-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tetraborato de sódio; Borax; Bórax

Special notes

When selecting the *Tetraborato de sódio* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tetraborato de sódio	9	13	33

Second-stage model

For differentiation of the substance/substance group *Tetraborato de sódio* the following second-stage model is used:

- Submodelo 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tetraborato de sódio* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	48,14	–
Fosfato dibásico de sódio di-hidratado	76,04	–
⋮	⋮	⋮
Citrato de magnésio	>50	56,34
Fosfato sódico de riboflavina hidratado	>50	59,83
Carbômero	>50	121,43
Sulfato de gentamicina	>50	128,64
Fosfato de Mg-Ca-K-colamina	>50	184,11
Gluconato de zinco	>50	195,85
Sulfato de tobramicina	>50	256,23
Sulfato de neomicina	>50	273,82
Finasterida	>50	1638,12

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tetraborato de sódio* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tetraborato de sódio*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tetraborato de sódio	13290118	21438	60	1412042
Caelo	Tetraborato de sódio	161372	22475	60	20160624*
Caelo	Tetraborato de sódio	161372	22621	40	20160624*
Euro OTC	Tetraborato de sódio	1404025-01	21656	60	20140514
Euro OTC	Tetraborato de sódio	1507024	21854	60	20150730*
Euro OTC	Tetraborato de sódio	1510032	22235	60	20151118*
Euro OTC	Tetraborato de sódio	1711002	23892	40	20171128*
Euro OTC	Tetraborato de sódio	2004009	25150	40	20200511*
Euro OTC	Tetraborato de sódio	2008006	25350	40	20200904*
Euro OTC	Tetraborato de sódio	2107002	25770	40	20210727*
Euro OTC	Tetraborato de sódio	2107002	25770SI	40	20210727*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 11 reference samples from the substance/substance group *Tetraborato de sódio*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 422 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 940 spectra of 23 reference samples from the substance/substance group *Tetraborato de sódio*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tetraborato de sódio	21000651002	25985	40
Caelo	Tetraborato de sódio	24000302	27244	40
Euro OTC	Tetraborato de sódio	1603043	22508	40
Euro OTC	Tetraborato de sódio	1607036	22713	40
Euro OTC	Tetraborato de sódio	1701046	22990	40
Euro OTC	Tetraborato de sódio	1804014	24093	40
Euro OTC	Tetraborato de sódio	2111003	25895	50
Euro OTC	Tetraborato de sódio	2202006	25944	40
Euro OTC	Tetraborato de sódio	2202007	25956	40
Euro OTC	Tetraborato de sódio	2202005	25968	40
Euro OTC	Tetraborato de sódio	2209019	26334	40
Euro OTC	Tetraborato de sódio	2307005	26885	40
Euro OTC	Tetraborato de sódio	2310017	27000	40
Caelo	Tetraborato de sódio	21000651002	25985SI	40
Caelo	Tetraborato de sódio	24000302	27244SI	40
Euro OTC	Tetraborato de sódio	2008006	25350SI†	40
Euro OTC	Tetraborato de sódio	2111003	25895SI	50

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetraborato de sódio	2202006	25944SI	40
Euro OTC	Tetraborato de sódio	2202007	25956SI	40
Euro OTC	Tetraborato de sódio	2202005	25968SI	40
Euro OTC	Tetraborato de sódio	2209019	26334SI	40
Euro OTC	Tetraborato de sódio	2307005	26885SI	40
Euro OTC	Tetraborato de sódio	2310017	27000SI	40

- 201 144 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 57 spectra from 44 *Apo-Ident* customers from 35 batches from the substance/substance group *Tetraborato de sódio*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tetraborato de sódio	2202006-01	1
	Tetraborato de sódio	2310017-01	1
	Tetraborato de sódio	2310017-02	2
Borax Francais	Tetraborato de sódio	1402002-01	1
Caelo	Tetraborato de sódio	11369412	1
Caelo	Tetraborato de sódio	11369431	1
Caelo	Tetraborato de sódio	1309032-01	1
Caelo	Tetraborato de sódio	13290118	1
Caelo	Tetraborato de sódio	14310905	2
Caelo	Tetraborato de sódio	150702401	1
Caelo	Tetraborato de sódio	1607036-01	1
Caelo	Tetraborato de sódio	16081801	1
Caelo	Tetraborato de sódio	16137201	1
Caelo	Tetraborato de sódio	16137205	1
Caelo	Tetraborato de sódio	21051402	1
Caesar & Loretz GmbH	Tetraborato de sódio	20000902001	1
EuRho	Tetraborato de sódio	1607036-01	2
Euro OTC	Tetraborato de sódio		1
Euro OTC	Tetraborato de sódio	130203401	1
Euro OTC	Tetraborato de sódio	1302034-01	1
Euro OTC	Tetraborato de sódio	1309032-01	1
Euro OTC	Tetraborato de sódio	13111207	1
Euro OTC	Tetraborato de sódio	1408006-01	1
Euro OTC	Tetraborato de sódio	1503043-01	1
Euro OTC	Tetraborato de sódio	1507024-01	3
Euro OTC	Tetraborato de sódio	160304301	1
Euro OTC	Tetraborato de sódio	1607036-01	2
Euro OTC	Tetraborato de sódio	1701046-01	1
Euro OTC	Tetraborato de sódio	1711002-01	8

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tetraborato de sódio	1804014-01	3
Euro OTC	Tetraborato de sódio	2004009-01	1
Euro OTC	Tetraborato de sódio	2008006-01	3
Euro OTC	Tetraborato de sódio	2107002-01	2
Euro OTC	Tetraborato de sódio	22020005-01	1
Euro/Alliance Healthcare	Tetraborato de sódio	171100201	1
Fagron	Tetraborato de sódio	12H09-N03	1
Gatt-Koller / Phoenix	Tetraborato de sódio	6187/01142114	1
Phoenix	Tetraborato de sódio	1603043-01	1
Sanacorp	Tetraborato de sódio	171100201	1

- 236 010 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tetraborato de sódio* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetraborato de sódio* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	940	0	201 144
Type C	0	57	0	236 010

The substance/substance group *Tetraborato de sódio* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3617 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 89.4737 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21438	21438	0,00	127,66
21656	22475	8,29	129,24
21854	21854	0,00	112,54
22235	22235	0,00	114,20
22475	22475	0,00	124,98
22621	22621	0,00	122,44
23892	23892	0,00	101,40
25150	25150	0,00	127,34
25350	25350	0,00	101,59
25770	25770	0,00	127,29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tetracaína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20947-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tetracaína; Tetracainum

Special notes

When selecting the *Tetracaína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tetracaína	9	13	161

Second-stage model

For differentiation of the substance/substance group *Tetracaína* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tetracaína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	152,18	–
⋮	⋮	⋮
Capsaicina	>50	116,99
Prednicarbato	>50	154,01
Acetato de ciproterona	>50	189,86
Cloridrato de oxibutinina	>50	197,97
Alfaestradiol	>50	223,11
Levocarnitina	>50	226,28
Citrato de sódio	>50	241,75
Cloridrato de amitriptilina	>50	252,29
Acetato de noretisterona	>50	349,52
Heparina sódica	>50	410,79
Piridoxal-5-fosfato	>50	500,87
Cloridrato de quinina di-hidratado	>50	535,08
Metoxisaleno	>50	590,00
Cloridrato de ciprofloxacina	>50	798,53
Valina	>50	1050,21
Amifampridina	>50	1510,72
Triclosan	>50	1768,56
Sacarose	>50	2140,85

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tetracaína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tetracaína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tetracaína	171117	23321	40	20170512*
Caelo	Tetracaína	181249	24255	40	20180605*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tetracaína	1405025-01	21603	60	AR-14-FG-012475-01
Euro OTC	Tetracaína	1512022	22299	45	20160128*
Euro OTC	Tetracaína	2304012	26661	40	20230508*
Fagron	Tetracaína	12L19-N10	20947	40	20130108
Fagron	Tetracaína	14A16-B04-292915	21650	60	20140205
Fagron	Tetracaína	14A16-B04-292916	21659	60	20140205
Fagron	Tetracaína	21L22-B01-216874	26081	40	20220315
Fagron	Tetracaína	21L22-B01-216874	26081SI	20	20220315

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 445 spectra of 10 reference samples from the substance/substance group *Tetracaína*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.
- 152 517 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 580 spectra of 16 reference samples from the substance/substance group *Tetracaína*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetracaína	1606009	22717	40
Euro OTC	Tetracaína	1609010	22858	40
Euro OTC	Tetracaína	1701035	23149	40
Euro OTC	Tetracaína	1708024	23736	40
Euro OTC	Tetracaína	1803002	24066	40
Euro OTC	Tetracaína	1805019	24135	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetracaína	1811021	24427	40
Euro OTC	Tetracaína	1903004	24451	40
Euro OTC	Tetracaína	1909021	24961	40
Euro OTC	Tetracaína	2107010	25883	50
Euro OTC	Tetracaína	2203018	26046	40
Euro OTC	Tetracaína	2308016	27071	40
Euro OTC	Tetracaína	2401016	27161	40
Euro OTC	Tetracaína	2107010	25883SI	10
Euro OTC	Tetracaína	2203018	26046SI	20
Euro OTC	Tetracaína	2304012	26661SI[†]	20

- 201 504 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 625 spectra from 230 *Apo-Ident* customers from 174 batches from the substance/substance group *Tetracaína*.
- Among them are spectra of independent samples from 160 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tetracaína	1811021-01	1
	Tetracaína	21L22-B01-216874	1
	Tetracaína	2203018-02	4
	Tetracaína	2302016-01	1
	Tetracaína	2304012-01	5
	Tetracaína	2304012-02	2
	Tetracaína	2401016-01	2
Caelo	Tetracaína	14A16-B04	1
Caelo	Tetracaína	14A16-B04-290207	1
Caelo	Tetracaína	14A16-B04-292916	1
Caelo	Tetracaína	1512022-01	1
Caelo	Tetracaína	1516B06312783	1
Caelo	Tetracaína	160004	1
Caelo	Tetracaína	1606009-01	1
Caelo	Tetracaína	16a13-b07-318736	1
Caelo	Tetracaína	16A13-B07-318736	5
Caelo	Tetracaína	16E23-B04	1
Caelo	Tetracaína	1701035-01	1
Caelo	Tetracaína	171111706	1
Caelo	Tetracaína	17111705	1
Caelo	Tetracaína	17111706	5
Caelo	Tetracaína	17111713	2
Caelo	Tetracaína	17111713P-190909-1	1
Caelo	Tetracaína	17111714	3
Caelo	Tetracaína	17K13-B02-344448	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracaína	17K13-B02-347172	2
Caelo	Tetracaína	1803002-01	1
Caelo	Tetracaína	1805019-01	2
Caelo	Tetracaína	1811021-01	2
Caelo	Tetracaína	18124097	1
Caelo	Tetracaína	18124905	1
Caelo	Tetracaína	19106602	5
Caelo	Tetracaína	19106605	1
Caelo	Tetracaína	192737004	3
Caelo	Tetracaína	192737006	1
Caelo	Tetracaína	192737008	1
Caelo	Tetracaína	20000160003	1
Caelo	Tetracaína	20000160009	2
Caelo	Tetracaína	20000160011	1
Caelo	Tetracaína	20003786004	2
Caelo	Tetracaína	20003786007	1
Caelo	Tetracaína	20003786012	8
Caelo	Tetracaína	2203018-01	2
Caelo	Tetracaína	T-290413-1	1
Caelo	Tetracaína	TC130621	1
Caeolo/Alliance	Tetracaína	20000160009	1
Caesar & Loretz GmbH...	Tetracaína	17111714	1
Caesar & Loretz GmbH...	Tetracaína	20000160003	1
Caesar & Loretz GmbH...	Tetracaína	17111706	1
Caesar & Loretz GmbH...	Tetracaína	20000160003	2
Caesar & Loretz GmbH	Tetracaína	18124906	1
Caesar & Loretz GmbH	Tetracaína	19106602	1
Caesar & Loretz GmbH	Tetracaína	192737004	1
Caesar & Loretz GmbH	Tetracaína	192737006	1
Caesar & Loretz GmbH	Tetracaína	20000160009	1
Caesar & Loretz GmbH	Tetracaína	20003786004	12
Caesar & Loretz GmbH	Tetracaína	20003786007	1
Caesar & Loretz/Noweda	Tetracaína	17111714	1
Ebert-Jacobi	Tetracaína	16J12-B06-327371	1
EuRho/ NOWEDA	Tetracaína	1811021-01	1
EuRho/ NOWEDA	Tetracaína	1903004-01	2
EuRho/ Phoenix	Tetracaína	1805019-01	1
EuRho/ Phoenix	Tetracaína	TC0090717	1
EuRho/AHD	Tetracaína	1811021-01	1
EuRho/GEHE	Tetracaína	1803002-01	1
EuRho/Jenne	Tetracaína	1909021-02	1
Eurho/noweda	Tetracaína	220301801	1
EuRho/Phoenix	Tetracaína	1909021-02	1
Eurho/Phönix	Tetracaína	1909021-01	1
EuRho	Tetracaína	220301801	1
EuRho	Tetracaína	519Q-04004	1
Euro OTC	Tetracaína	10887133	1
Euro OTC	Tetracaína	12081501	1
Euro OTC	Tetracaína	1312034-01	6
Euro OTC	Tetracaína	1405025-01	1
Euro OTC	Tetracaína	1405025-02	1
Euro OTC	Tetracaína	151022-01	1
Euro OTC	Tetracaína	1512022-01	4
Euro OTC	Tetracaína	160600-01	1
Euro OTC	Tetracaína	1606009-01	7
Euro OTC	Tetracaína	160901	1
Euro OTC	Tetracaína	1609010-01	15
Euro OTC	Tetracaína	1701035-01	10
Euro OTC	Tetracaína	170802401	3
Euro OTC	Tetracaína	1708024-01	12

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tetracaína	1803002-01	16
Euro OTC	Tetracaína	18041809	1
Euro OTC	Tetracaína	180501901	2
Euro OTC	Tetracaína	1805019-01	10
Euro OTC	Tetracaína	1805019-02	2
Euro OTC	Tetracaína	181102101	8
Euro OTC	Tetracaína	1811021-01	29
Euro OTC	Tetracaína	19009021-02	1
Euro OTC	Tetracaína	1903001-02	1
Euro OTC	Tetracaína	1903004	2
Euro OTC	Tetracaína	190300401	1
Euro OTC	Tetracaína	1903004-01	22
Euro OTC	Tetracaína	1903004-02	3
Euro OTC	Tetracaína	1903004-03	2
Euro OTC	Tetracaína	1909021-01	33
Euro OTC	Tetracaína	1909021-02	1
Euro OTC	Tetracaína	1909021-21	2
Euro OTC	Tetracaína	19K04-F07	1
Euro OTC	Tetracaína	19K04-F07-368617	1
Euro OTC	Tetracaína	2107010-01	26
Euro OTC	Tetracaína	2203018-01	26
Euro OTC	Tetracaína	2203018-02	17
Euro OTC	Tetracaína	2203018-16	1
Euro OTC	Tetracaína	2304012-01	2
Euro OTC	Tetracaína	3081701	1
Euro OTC	Tetracaína	TC0010118	1
Euro OTC	Tetracaína	TC0041018	1
Euro OTC	Tetracaína	TC0091115	1
Euro/Noweda	Tetracaína	1805019-01	2
Euro/Phönix	Tetracaína	1903004-02	1
Fag	Tetracaína	16A13-B07-322947	1
Fagro/Noweda	Tetracaína	19A15-B01-361269	1
Fagron	Tetracaína		2
Fagron	Tetracaína	11D07-N20	1
Fagron	Tetracaína	11G12-N13	3
Fagron	Tetracaína	11l01-N09	1
Fagron	Tetracaína	11L09-N03	3
Fagron	Tetracaína	12F26-NO5	1
Fagron	Tetracaína	12f29-n05	1
Fagron	Tetracaína	12F29-N05	7
Fagron	Tetracaína	12H23-N07	1
Fagron	Tetracaína	12L19-N10	5
Fagron	Tetracaína	13D30-N11	2
Fagron	Tetracaína	14A16-B04	1
Fagron	Tetracaína	14A16-B04-2490207	1
Fagron	Tetracaína	14a16-b04-290208	1
Fagron	Tetracaína	14A16-B04-290208	3
Fagron	Tetracaína	14A16-B04-290209	1
Fagron	Tetracaína	14A16-B04-292916	1
Fagron	Tetracaína	14G30-B08	2
Fagron	Tetracaína	14g30-b08-297305	1
Fagron	Tetracaína	14G30-B08-297305	1
Fagron	Tetracaína	14g30-b08-297306	1
Fagron	Tetracaína	14G30-B08-297306	2
Fagron	Tetracaína	14G30-B08-297307	1
Fagron	Tetracaína	14K03-B02	1
Fagron	Tetracaína	14K03B02303178	1
Fagron	Tetracaína	14K03-B02-303178	1
Fagron	Tetracaína	14K03-B02-303179	2
Fagron	Tetracaína	15/16-B06-312783	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tetracaína	15/16-B06-316260	1
Fagron	Tetracaína	1516-B06-316259	1
Fagron	Tetracaína	1516-B06-316260	1
Fagron	Tetracaína	15D01-B03-306258	3
Fagron	Tetracaína	15G30-B04-312060	1
Fagron	Tetracaína	16A13-B07-318736	5
Fagron	Tetracaína	16A13-B07-322947	2
Fagron	Tetracaína	16E23-B04-323269	1
Fagron	Tetracaína	16G29-B02-325569	4
Fagron	Tetracaína	16G29B02325570	2
Fagron	Tetracaína	16G29-B02-325570	1
Fagron	Tetracaína	16J12-B06	1
Fagron	Tetracaína	16J12-B06-327371	1
Fagron	Tetracaína	16J12-B06-329087	2
Fagron	Tetracaína	17184083	2
Fagron	Tetracaína	17E18-B02-337216	3
Fagron	Tetracaína	17E18-B02-337217	2
Fagron	Tetracaína	17K13-B02	1
Fagron	Tetracaína	17K13-B02-34172	1
Fagron	Tetracaína	17K13-B02-344448	7
Fagron	Tetracaína	17K13-B02-347172	7
Fagron	Tetracaína	18104050	1
Fagron	Tetracaína	18C26-B01-350472	1
Fagron	Tetracaína	19A15-B01	2
Fagron	Tetracaína	19A15-B010	2
Fagron	Tetracaína	19A15-B01-361263	2
Fagron	Tetracaína	19A15-B01-361269	5
Fagron	Tetracaína	19K04-F0-366996	1
Fagron	Tetracaína	19K04-F07	2
Fagron	Tetracaína	19K04-F07-0366996	1
Fagron	Tetracaína	19K04-F07-366996	4
Fagron	Tetracaína	19K04-F07-3669966	1
Fagron	Tetracaína	19K04-F07-368617	2
Fagron	Tetracaína	19K04-F07-369725	2
Fagron	Tetracaína	20E20-F06	3
Fagron	Tetracaína	20E20-F06-371444	3
Fagron	Tetracaína	20H28-U01-009031	1
Fagron	Tetracaína	20K16-F03-376067	1
Fagron	Tetracaína	2107070-01	2
Fagron	Tetracaína	21G10-B23-213654	1
Fagron	Tetracaína	21G10-B23-216782	4
Fagron	Tetracaína	21L22-B01-215564	4
Fagron	Tetracaína	21L22-B01-216874	1
Fagron	Tetracaína	2203018-02	3
Fagron	Tetracaína	2913Q-07165	1
Fagron	Tetracaína	3465093	1
Fagron	Tetracaína	5111202	1
Fagron	Tetracaína	9K04-F07-369725	1
Fagron	Tetracaína	F07-3697205	1
Fagron	Tetracaína	TC0041018	1
Fagron	Tetracaína	TC0070716	1
Fagron	Tetracaína	TC0090913	2
Fagron	Tetracaína	TC0140719	2
Fargon/AHD	Tetracaína	17K13-B02-347172	1
Fargon/Gehe	Tetracaína	18C26-B01-350472	1
Fargon/Gehe	Tetracaína	18c26-B01-355789	1
Fragon/ Gehe	Tetracaína	18C26-B01-350472	1
Fragon/ Phönix	Tetracaína	19a15b01361263	1
GEHE 02.05.2014	Tetracaína	14A16-B04-290208	2
GEHE 04.05	Tetracaína	1405025-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
GEHE	Tetracaína	16G29-B02-325569	1
Gehe	Tetracaína	170103501	1
Gehe	Tetracaína	1805019-01	2
Gehe	Tetracaína	1811021-01	1
GEHE	Tetracaína	18C26-B01	1
Gehe	Tetracaína	21L22-B01-222760	1
gehe	Tetracaína	21L22-B01-222760	2
Gehe	Tetracaína	2304012-01	1
Gehe-Berlin	Tetracaína	2401016-01	2
Geilenkirchen	Tetracaína	1805019-01	2
Hepart	Tetracaína	15G30-B04-310590	1
Jenne	Tetracaína	2203018-02	1
Noweda, EuRho	Tetracaína	2203018-01	1
Noweda/Fargon	Tetracaína	16/12-B06-329087	1
Noweda	Tetracaína	19A15-B01-361269	3
Phoenix 07.10.14	Tetracaína	14A16-B04-292916	1
Phoenix Goettin	Tetracaína	14G30-B08-297306	1
phoenix	Tetracaína	14A16B04290207	2
Phoenix	Tetracaína	1811021-01	1
Phoenix	Tetracaína	19k04-f07366996	1
Phoenix	Tetracaína	19k04-f07-366996	1
Phoenix	Tetracaína	19k04-f07369725	1
Phoenix	Tetracaína	20e20-f06-371444	1
Phoenix	Tetracaína	3118	1
Phönix Gotha	Tetracaína	10F11N04	1
Phönix	Tetracaína	11g12-n13	1
Phönix	Tetracaína	1303018-01	1
Phönix	Tetracaína	1312034-01	2
Phönix	Tetracaína	1708024-01	2
PHÖNIX	Tetracaína	20003786004	1
Phönix	Tetracaína	2304012-01	1
Phönix	Tetracaína	3465093	1
Rondell Apotheke	Tetracaína	1312034-01	1
Sanacorp	Tetracaína	1803002-01	1
Sanacorp	Tetracaína	1805019-01	1
sanacorp	Tetracaína	2203018-02	1
Sanacorp	Tetracaína	2304012-01	1
Sanacorp	Tetracaína	2308016-01	2
Sanacorp	Tetracaína	F07-3669906	1
Siegfried / Gehe	Tetracaína	18C26-B01-350472	1
siehe Lennartz	Tetracaína	sieheLennartz	1
tetracain	Tetracaína	1903004-03	1

- 235 442 spectra from 1515 *Apo-Ident* customers from a total of 49 087 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tetracaína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracaína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	445	0	152 517
Type B	0	580	0	201 504
Type C	0	625	0	235 442

The substance/substance group *Tetracaína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6517 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9655 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.0400 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20947	21603	10,06	163,24
21603	21603	0,00	161,77
21650	22299	6,24	164,77
21659	21603	7,04	165,13
22299	22299	0,00	164,86
23321	23321	0,00	165,00
24255	24255	0,00	164,16
26081	24255	10,86	164,23
26661	26661	0,00	162,03

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Timerosal**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20702-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Timerosal; Thiomersalum

Special notes

When selecting the *Timerosal* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Timerosal	3	1	13

Second-stage model

For differentiation of the substance/substance group *Timerosal* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Timerosal* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de prilocaína	98,29	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Timerosal* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Timerosal*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Timerosal	172173	23679	30	20170919*
Caelo	Timerosal	22003780	27219	40	20230404*
Caelo	Timerosal	22003780	27219SI	20	20230404*
Fagron	Timerosal	11K01-N03	20702	40	1401417

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 130 spectra of 4 reference samples from the substance/substance group *Timerosal*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 832 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Timerosal*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Timerosal	193090	25198	40

- 202 044 spectra from a total of 4044 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 13 *Apo-Ident* customers from 14 batches from the substance/substance group *Timerosal*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Timerosal	22003780001	1
	Timerosal	22003780002	1
	Timerosal	23003535001	2
Caelo	Timerosal	10296413	1
Caelo	Timerosal	13577020	1
Caelo	Timerosal	20004306001	1
Caelo	Timerosal	20004306002	1
Caelo	Timerosal	20004306003	2
Caelo	Timerosal	21051507	1
Caesar & Loretz GmbH	Timerosal	12275218	1
Caesar & Loretz GmbH	Timerosal	193090002	1
Caesar & Loretz GmbH	Timerosal	20004306003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Timerosal		1
Fagron	Timerosal	12F19-N11	1
Fagron	Timerosal	12J17-N02	1

- 236 050 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Timerosal* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Timerosal* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	130	0	152 832
Type B	0	40	0	202 044
Type C	0	17	0	236 050

The substance/substance group *Timerosal* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20702	20702	0,00	134,87
23679	23679	0,00	140,08
27219	27219	0,00	133,94

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Timol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20003-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Timol; Thymolum

Special notes

When selecting the *Timol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Timol	8	9	79

Second-stage model

For differentiation of the substance/substance group *Timol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Timol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mentol	79,70	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Timol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Timol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Timol	14025805	21469	60	20140127
Caelo	Timol	16144101	23160	40	20160606
Caelo	Timol	173407	23837	40	20180110*
Caelo	Timol	21000880	25650	40	20210401*
Caelo	Timol	23001568	26840	40	20230622*
Caelo	Timol	23001568	26840SI	40	20230622*
Euro OTC	Timol	1312022-02	21639	60	20131219
Euro OTC	Timol	1510004	21943	60	20151016*
Fagron	Timol	15H13-B05-328912	23499	40	20151118

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 9 reference samples from the substance/substance group *Timol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 152 542 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 409 spectra of 11 reference samples from the substance/substance group *Timol*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Timol	181424	24231	40
Caelo	Timol	190342	24552	40
Caelo	Timol	21002863	25862	50
Caelo	Timol	22002344	26245	40
Caelo	Timol	22002044	26258	40
Caelo	Timol	24000390	27122	40
Caelo	Timol	24001437	27313	39
Euro OTC	Timol	1710037	23773	40
Euro OTC	Timol	1808014	24299	40
Caelo	Timol	22002344	26245SI	20
Caelo	Timol	22002044	26258SI	20

- 201 675 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 234 spectra from 180 *Apo-Ident* customers from 82 batches from the substance/substance group *Timol*.
- Among them are spectra of independent samples from 79 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Timol	14025802	1
	Timol	22002044004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Timol	23000600003	1
ACM / Herba	Timol	KNC1166J14	1
Alliance Healthcare	Timol	20003672009	1
apo-ident	Timol	1808014-01	1
Caelo	Timol	11178718	1
Caelo	Timol	11358607	2
Caelo	Timol	11358608	1
Caelo	Timol	11358616	2
Caelo	Timol	13147502	2
Caelo	Timol	13288802	4
Caelo	Timol	13288806	1
Caelo	Timol	14025802	2
Caelo	Timol	14025805	1
Caelo	Timol	14025807	1
Caelo	Timol	14025809	2
Caelo	Timol	14025815	1
Caelo	Timol	14025816	1
Caelo	Timol	14302401	1
Caelo	Timol	14310601	2
Caelo	Timol	14310605	1
Caelo	Timol	15130101	2
Caelo	Timol	15130106	3
Caelo	Timol	15362901	5
Caelo	Timol	15362908	4
Caelo	Timol	16144101	6
Caelo	Timol	16144105	7
Caelo	Timol	16144108	7
Caelo	Timol	161441108	1
Caelo	Timol	1730711	1
Caelo	Timol	17324203	4
Caelo	Timol	17340708	1
Caelo	Timol	17340711	7
Caelo	Timol	17340716	2
Caelo	Timol	18221907	1
Caelo	Timol	19034203	5
Caelo	Timol	19034205	4
Caelo	Timol	19061303	1
Caelo	Timol	192437003	3
Caelo	Timol	19243701	9
Caelo	Timol	20001482001	6
Caelo	Timol	20001482003	5
Caelo	Timol	20003672003	3
Caelo	Timol	20003672006	6
Caelo	Timol	20003672007	5
Caelo	Timol	20003750002	1
Caelo	Timol	2031503	1
Caelo	Timol	21000880002	2
Caelo	Timol	21000880007	2
Caelo	Timol	2100088002	1
Caelo	Timol	21042	1
Caelo	Timol	4364887223	1
Caesar & Loretz GmbH...	Timol	19034205	1
Caesar & Loretz GmbH...	Timol	21000880009	1
Caesar & Loretz GmbH...	Timol	19034203	1
Caesar & Loretz GmbH...	Timol	192437003	1
Caesar & Loretz GmbH...	Timol	18221907	1
Caesar & Loretz GmbH...	Timol	20003672009	1
Caesar & Loretz GmbH	Timol	16144101	1
Caesar & Loretz GmbH	Timol	17340711	1
Caesar & Loretz GmbH	Timol	17340716	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Timol	19034203	1
Caesar & Loretz GmbH	Timol	19034205	1
Caesar & Loretz GmbH	Timol	192437003	1
Caesar & Loretz GmbH	Timol	19243701	3
Caesar & Loretz GmbH	Timol	20001482001	2
Caesar & Loretz GmbH	Timol	20003672003	3
Caesar & Loretz GmbH	Timol	20003672006	2
Caesar & Loretz GmbH	Timol	20003672007	2
Caesar & Loretz GmbH	Timol	20003750002	1
Caesar & Loretz GmbH	Timol	21000880005	1
Caesar & Loretz GmbH	Timol	21000880007	1
Caesar § Lorenz GmbH	Timol	13288806	1
Ebert & Jacobi 02...	Timol	15362901	1
Euro OTC	Timol	1107021-01	1
Euro OTC	Timol	11358603	1
Euro OTC	Timol	1202028-01	1
Euro OTC	Timol	1312022-01	1
Euro OTC	Timol	1410007-01	5
Euro OTC	Timol	15100004-03	1
Euro OTC	Timol	1510004-01	2
Euro OTC	Timol	1510004-02	9
Euro OTC	Timol	1510004-03	1
Euro OTC	Timol	1710037-01	5
Euro OTC	Timol	1808014-01	3
Euro OTC	Timol	20151012-1	1
Euro/ Phönix	Timol	1510004-02	1
Euro/Phönix	Timol	180801401	1
Fagron	Timol	12B06-N11	1
Fagron	Timol	12E30-N11	1
Fagron	Timol	12H29-N02	2
Fagron	Timol	12K01-N02	2
Fagron	Timol	12M29-N02	1
Fagron	Timol	713575	1
Fagron	Timol	8G23-N09	2
Frey+Lau GmbH/Phönix	Timol	1312022-01	1
Gehe Kassel	Timol	1312022-01	1
gehe	Timol	1808014-01	1
Gehe	Timol	19243701	1
gehe	Timol	20003672003	1
gehe	Timol	5112139	1
L12	Timol	15172002	1
L30	Timol	1510004-03	1
Noweda	Timol	12k01-no2	1
Noweda	Timol	16144105	1
Noweda	Timol	20003750007	2
PHOENIX 26.03.2014	Timol	14025802	2
Phoenix	Timol	19034205	1
Phoenix	Timol	20001482003	1
Phönix	Timol	11358610	1
Phönix	Timol	1510004-01	1
Phönix	Timol	20001482003	1
Sanacorp	Timol	1135816	1
Sanacorp	Timol	9E14-N16	1
xxxxx	Timol		1
xxxxx	Timol	RT1211	1

- 235 833 spectra from 1515 *Apo-Ident* customers from a total of 49 177 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Timol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Timol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	409	0	201 675
Type C	0	234	0	235 833

The substance/substance group *Timol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5330 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.4359 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21469	23837	13,96	123,17
21639	23837	10,94	122,78
21943	21943	0,00	127,80
23160	23837	17,58	122,64
23499	23837	7,33	124,42
23837	23837	0,00	123,41
25650	25650	0,00	122,63
26840	26840	0,00	118,32

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tirosina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	21574-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tirosina; Tyrosinum

Special notes

When selecting the *Tirosina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tirosina	6	3	5

Second-stage model

For differentiation of the substance/substance group *Tirosina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tirosina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	108,30	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tirosina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tirosina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tirosina	2204019	26095	40	20220519*
Euro OTC	Tirosina	2204019	26095SI	20	20220519*
Fagron	Tirosina	13G24-N22	21574	60	1411030
Fagron	Tirosina	16B26-B01-322911	23533	40	20160324
Fagron	Tirosina	18E15-B02-359934	24692	40	20181001
Fagron	Tirosina	22B07-B15-221081	26166	40	20220602
Fagron	Tirosina	22B07-B15-221081	26166SI	20	20220602
Fagron	Tirosina	22H12-B03-222150	26388	40	20220927
Fagron	Tirosina	22H12-B03-222150	26388SI	20	20220927

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 320 spectra of 9 reference samples from the substance/substance group *Tirosina*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 130 spectra of 3 reference samples from the substance/substance group *Tirosina*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tirosina	17B06-B03-338139	24008	40
Fagron	Tirosina	19I20-F02-365384	25749	50
Fagron	Tirosina	23B21-B03-227898	27024	40

- 201 954 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Tirosina*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Tirosina	2204019-01	1
Euro OTC	Tirosina	L1210050-01	1
Euro OTC	Tirosina	L1401037	1
Euro OTC	Tirosina	L1506022-02	1
Euro OTC	Tirosina	L1506022-05	1

- 236 062 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tirosina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tirosina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	130	0	201 954
Type C	0	5	0	236 062

The substance/substance group *Tirosina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21574	21574	0,00	197,64
23533	26095	8,08	204,17
24692	26095	13,56	207,82
26095	26095	0,00	205,38
26166	26095	14,84	209,73
26388	26095	14,78	209,30

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tirotricina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20732-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tirotricina; Tyrothricinum

Special notes

When selecting the *Tirotricina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tirotricina	3	2	16

Second-stage model

For differentiation of the substance/substance group *Tirotricina* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tirotricina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Gramicidina	55,49	49,09
⋮	⋮	⋮
Metilprednisolona	>50	71,34
Fluocinolona acetonida	>50	85,25
Betametasona	>50	98,74
Triancinolona acetonido	>50	105,21
Prednisolona	>50	111,50
Dexametasona	>50	131,65

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tirotricina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tirotricina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tirotricina	12K14-N01	20732	40	1509178
Fagron	Tirotricina	12K14-N01	21683	60	AR-15-FG-001172-01
Fagron	Tirotricina	14A23-B05-294146	21876	60	AR-15-FG-015005-01
Fagron	Tirotricina	19C05-B01-370262	25183	40	20200511

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 200 spectra of 4 reference samples from the substance/substance group *Tirotricina*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 152 762 spectra from a total of 2839 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Tirotricina*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tirotricina	17E09-B03-341231	23742	40
Fagron	Tirotricina	20L15-F03-376267	26066	40
Fagron	Tirotricina	20L15-F03-376267	26066SI	10

- 201 994 spectra from a total of 4043 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 30 spectra from 21 *Apo-Ident* customers from 18 batches from the substance/substance group *Tirotricina*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Tirotricina	13A14-N04	1
Fagron	Tirotricina	15A06-B02-3005	1
Fagron	Tirotricina	15A06-B02-303893	1
Fagron	Tirotricina	15a06-B02-323005	1
Fagron	Tirotricina	15A06-B02-323005	5
Fagron	Tirotricina	17E09-B03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tirotricina	17E09-B03-341231	2
Fagron	Tirotricina	17E09-B03-350209	1
Fagron	Tirotricina	17E09-B03-351982	1
Fagron	Tirotricina	17E09B03352743	1
Fagron	Tirotricina	17E09-B03-352743	5
Fagron	Tirotricina	17E09-B03-355400	1
Fagron	Tirotricina	19C05-B01370262	1
Fagron	Tirotricina	19C05-B01-370262	1
Fagron	Tirotricina	19C05-B01-370998	3
Fagron	Tirotricina	B2500226	2
Parthe Apotheke	Tirotricina	171/19	1
Sanacorp	Tirotricina	20L15-F03-376267	1

- 236 037 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tirotricina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tirotricina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	90	0	201 994
Type C	0	30	0	236 037

The substance/substance group *Tirotricina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 80.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20732	20732	0,00	96,96
21683	21683	0,00	96,85
21876	21876	0,00	90,87
25183	21876	12,97	91,97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tosilcloramida sódica**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20133-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tosilcloramida sódica; Tosylchloramidum natricum

Special notes

When selecting the *Tosilcloramida sódica* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tosilcloramida sódica	4	3	36

Second-stage model

For differentiation of the substance/substance group *Tosilcloramida sódica* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tosilcloramida sódica* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	67,09	–
⋮	⋮	⋮
Riboflavina	>50	26,67
Sulfato de polimixina B	>50	53,63
Bromidrato de hioscina	>50	62,39
Bacitracina	>50	68,00
Cianocobalamina	>50	69,16
Sulfato de colistina	>50	71,78
Anfotericina B	>50	90,29
Pantotenato de cálcio	>50	103,14
Estradiol hemi-hidratado	>50	124,25
Nistatina	>50	124,33
Glicerofosfato de cálcio	>50	133,41
Triancinolona	>50	144,65
Estriol	>50	157,90
SyrSpend® SF pH4 neo	>50	178,05
Vitamina E acetato pó 50%	>50	178,13
Metilcobalamina	>50	180,89
Levedura de selênio	>50	196,45
Ácido oxálico	>50	202,95
Gelatina, branca	>50	203,25
SyrSpend® SF Alka	>50	205,50
Amido de arroz	>50	222,79
Carmelose sódica	>50	272,25
Amido de trigo	>50	291,07
Frutose	>50	308,09
SyrSpend® SF pH4	>50	318,73
Fécula de batata	>50	341,64
Amido de milho	>50	387,86
Goma arábica, dispersão seca	>50	399,91
Maltodextrina	>50	431,45

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tosilcloramida sódica* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tosilcloramida sódica*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tosilcloramida sódica	13103201	20864	40	20130424
Caelo	Tosilcloramida sódica	13361602	21115	40	1407634
Caelo	Tosilcloramida sódica	16236603	23562	40	20160819
Caelo	Tosilcloramida sódica	172265	24238	40	20170906*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Tosilcloramida sódica*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 802 spectra from a total of 2838 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Tosilcloramida sódica*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tosilcloramida sódica	13361606	21480	60
Caelo	Tosilcloramida sódica	162366	22773	40
Caelo	Tosilcloramida sódica	23000577	27114	40
Caelo	Tosilcloramida sódica	23000577	27114SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 924 spectra from a total of 4042 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 93 spectra from 58 *Apo-Ident* customers from 37 batches from the substance/substance group *Tosilcloramida sódica*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tosilcloramida sódica	89539524	1
Anzag	Tosilcloramida sódica	12H09-N01	1
Caelo	Tosilcloramida sódica	11116708	1
Caelo	Tosilcloramida sódica	12277005	3
Caelo	Tosilcloramida sódica	12323605	1
Caelo	Tosilcloramida sódica	12323606	1
Caelo	Tosilcloramida sódica	12323607	1
Caelo	Tosilcloramida sódica	12323609	2
Caelo	Tosilcloramida sódica	1310206	1
Caelo	Tosilcloramida sódica	13103206	8
Caelo	Tosilcloramida sódica	13103207	1
Caelo	Tosilcloramida sódica	13103210	2
Caelo	Tosilcloramida sódica	13361606	4
Caelo	Tosilcloramida sódica	13361607	6
Caelo	Tosilcloramida sódica	14183504	1
Caelo	Tosilcloramida sódica	14183509	1
Caelo	Tosilcloramida sódica	15039603	4
Caelo	Tosilcloramida sódica	15183905	1
Caelo	Tosilcloramida sódica	15370501	5
Caelo	Tosilcloramida sódica	15370505	2
Caelo	Tosilcloramida sódica	16236603	11
Caelo	Tosilcloramida sódica	16236603/1180117	1
Caelo	Tosilcloramida sódica	16236607	6
Caelo	Tosilcloramida sódica	16236611	3
Caelo	Tosilcloramida sódica	17061503	3
Caelo	Tosilcloramida sódica	17061511	1
Caelo	Tosilcloramida sódica	17226502	2
Caelo	Tosilcloramida sódica	17226503	4
Caelo	Tosilcloramida sódica	71051187	2
Caelo	Tosilcloramida sódica	72215377	2
Caeolo	Tosilcloramida sódica	16236607	1
EuRho	Tosilcloramida sódica	133610607	1
Fagron	Tosilcloramida sódica	11L08-N04	1
Fagron	Tosilcloramida sódica	14B27-B03-291967	1
Fagron	Tosilcloramida sódica	14L12-B01-301915	1
Hydra International Ltd	Tosilcloramida sódica	91020132	1
L10	Tosilcloramida sódica	16236607	2
Lysoform	Tosilcloramida sódica	K-09-2019	1
Sanacorp	Tosilcloramida sódica	12H09-N01	1
Taoasis	Tosilcloramida sódica	1623607	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 235 974 spectra from 1515 *Apo-Ident* customers from a total of 49 222 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tosilcloramida sódica* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tosilcloramida sódica* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	160	0	201 924
Type C	0	93	0	235 974

The substance/substance group *Tosilcloramida sódica* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.5484 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20864	21115	21,06	152,61
21115	21115	0,00	144,74
23562	21115	16,88	150,77
24238	24238	0,00	151,76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tretinoína**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20474-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tretinoína; Ácido retinoico; Tretinoinum

Special notes

When selecting the *Tretinoína* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tretinoína	6	18	333

Second-stage model

For differentiation of the substance/substance group *Tretinoína* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tretinoína* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de mepivacaína	69,10	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tretinoína* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tretinoína*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tretinoína	15028403	21757	60	1507086
Caelo	Tretinoína	15028403	21757SI	60	1507086
Caelo	Tretinoína	15239503	21878	60	20150717
Caelo	Tretinoína	15239503	21878SI	60	20150717
Euro OTC	Tretinoína	1402007-02	21747	60	1507085
Euro OTC	Tretinoína	1402007-02	21747SI	60	1507085
Euro OTC	Tretinoína	1510007	21940	60	20151102*
Euro OTC	Tretinoína	1510007	21940SI	60	20151102*
Euro OTC	Tretinoína	1604059	22574	40	20160603*
Fagron	Tretinoína	15F01-B06-317884	22936	40	20150619
Fagron	Tretinoína	15F01-B06-317884	22936SI	40	20150619

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 600 spectra of 11 reference samples from the substance/substance group *Tretinoína*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 362 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1460 spectra of 37 reference samples from the substance/substance group *Tretinoína*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tretinoína	162915	22779	40
Caelo	Tretinoína	162171	22780	40
Caelo	Tretinoína	172731	23680	40
Caelo	Tretinoína	173057	23843	40
Caelo	Tretinoína	181673	24251	40
Caelo	Tretinoína	181674	24258	40
Euro OTC	Tretinoína	1612010	22911	40
Euro OTC	Tretinoína	1804005	24061	40
Euro OTC	Tretinoína	1901001	24456	40
Euro OTC	Tretinoína	1907014	24855	40
Euro OTC	Tretinoína	2004014	25283	40
Euro OTC	Tretinoína	2106017	25779	40
Euro OTC	Tretinoína	2205021	26228	40
Euro OTC	Tretinoína	2303017	26655	40
Euro OTC	Tretinoína	2311013	27198	40
Euro OTC	Tretinoína	2406007	27407	40
Fagron	Tretinoína	18J30-B02-358547	24824	40
Fagron	Tretinoína	22F28-B05-221065	26606	40
Caelo	Tretinoína	162915	22779SI	40
Caelo	Tretinoína	162171	22780SI	40
Caelo	Tretinoína	172731	23680SI	40
Caelo	Tretinoína	173057	23843SI	40
Caelo	Tretinoína	181673	24251SI	20
Caelo	Tretinoína	181674	24258SI	40
Euro OTC	Tretinoína	1604059	22574SI†	40
Euro OTC	Tretinoína	1612010	22911SI	40
Euro OTC	Tretinoína	1804005	24061SI	40
Euro OTC	Tretinoína	1901001	24456SI	40
Euro OTC	Tretinoína	1907014	24855SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tretinoína	2004014	25283SI	40
Euro OTC	Tretinoína	2106017	25779SI	40
Euro OTC	Tretinoína	2205021	26228SI	40
Euro OTC	Tretinoína	2303017	26655SI	40
Euro OTC	Tretinoína	2311013	27198SI	40
Euro OTC	Tretinoína	2406007	27407SI	40
Fagron	Tretinoína	18J30-B02-358547	24824SI	40
Fagron	Tretinoína	22F28-B05-221065	26606SI	40

- 200 624 spectra from a total of 4026 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1649 spectra from 729 *Apo-Ident* customers from 340 batches from the substance/substance group *Tretinoína*.

- Among them are spectra of independent samples from 332 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tretinoína	2004014-02	1
	Tretinoína	2100421009	1
	Tretinoína	21004211007	1
	Tretinoína	2106017-02	4
	Tretinoína	2106017-03	1
	Tretinoína	21G10-B08-213327	1
	Tretinoína	2205021-01	6
	Tretinoína	2205021-02	9
	Tretinoína	2205321-02	1
	Tretinoína	22120002	1
	Tretinoína	22F28-B05-221065	1
	Tretinoína	2303017	4
	Tretinoína	2303017-01	18
	Tretinoína	23A23-B12-225240	1
	Tretinoína	24000848003	1
AHC	Tretinoína	2205021-02	1
AHD	Tretinoína	16070002	1
AHD	Tretinoína	1901001-01	1
AHD	Tretinoína	1907014-02	1
AHD	Tretinoína	2311013-01	1
Alliance Healthcare	Tretinoína	20000490002	1
Alliance Healthcare	Tretinoína	2205021-01	1
Allianz Healthcare	Tretinoína	1907014-01	1
Anzag/Henry Lamotte	Tretinoína	15078303	1
Anzag	Tretinoína	14L24B01303157	1
Anzag	Tretinoína	15078305	1
Apo Ident/ Noweda	Tretinoína	1804005-01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
apo-ident	Tretinoína	1804005-01	1
Apo-ident	Tretinoína	2004014-01	1
apomix	Tretinoína	8806694	1
BASF / Phönix	Tretinoína	1604059-02	1
BASF	Tretinoína	1402007-03	1
Bombastus	Tretinoína	1402007-03	1
Caelo	Tretinoína		1
Caelo	Tretinoína	10003050032	1
Caelo	Tretinoína	1109014-02	1
Caelo	Tretinoína	11225504	1
Caelo	Tretinoína	11225506	1
Caelo	Tretinoína	11225511	1
Caelo	Tretinoína	11284703	1
Caelo	Tretinoína	12023302	9
Caelo	Tretinoína	12023303	1
Caelo	Tretinoína	12023309	1
Caelo	Tretinoína	12102902	1
Caelo	Tretinoína	12102903	2
Caelo	Tretinoína	12102904	2
Caelo	Tretinoína	12320201	2
Caelo	Tretinoína	12320203	2
Caelo	Tretinoína	12320204	1
Caelo	Tretinoína	12320205	5
Caelo	Tretinoína	12320207	1
Caelo	Tretinoína	12320209	6
Caelo	Tretinoína	12320301	1
Caelo	Tretinoína	12320303	1
Caelo	Tretinoína	12367101	2
Caelo	Tretinoína	12367103	2
Caelo	Tretinoína	12367104	1
Caelo	Tretinoína	12959AX20	1
Caelo	Tretinoína	12D05-N08	1
Caelo	Tretinoína	12I06-N01	1
Caelo	Tretinoína	1304028-02	3
Caelo	Tretinoína	131950002	1
Caelo	Tretinoína	13195002	14
Caelo	Tretinoína	13195003	1
Caelo	Tretinoína	13195008	1
Caelo	Tretinoína	13278101	1
Caelo	Tretinoína	13278102	4
Caelo	Tretinoína	13278104	2
Caelo	Tretinoína	13278105	2
Caelo	Tretinoína	13308003	1
Caelo	Tretinoína	13308004	4
Caelo	Tretinoína	13B05-B02-287360	1
Caelo	Tretinoína	14040504	5
Caelo	Tretinoína	14040507	1
Caelo	Tretinoína	14093502	4
Caelo	Tretinoína	14093503	1
Caelo	Tretinoína	1411016-01	2
Caelo	Tretinoína	14252702	5
Caelo	Tretinoína	14252706	2
Caelo	Tretinoína	14252710	2
Caelo	Tretinoína	14252801	1
Caelo	Tretinoína	1452802	1
Caelo	Tretinoína	14L24-B01-303157	2
Caelo	Tretinoína	15078301	1
Caelo	Tretinoína	15078302	2
Caelo	Tretinoína	15078303	2
Caelo	Tretinoína	15078305	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tretinoína	15078307	3
Caelo	Tretinoína	15078308	1
Caelo	Tretinoína	151000701	1
Caelo	Tretinoína	1510007-02	2
Caelo	Tretinoína	1517E-02563	1
Caelo	Tretinoína	15239501	2
Caelo	Tretinoína	15239502	6
Caelo	Tretinoína	15239503	2
Caelo	Tretinoína	15437301	1
Caelo	Tretinoína	15437303	14
Caelo	Tretinoína	15F01-B06-308856	1
Caelo	Tretinoína	15H31-B01	1
Caelo	Tretinoína	160405901	1
Caelo	Tretinoína	1604059-02	1
Caelo	Tretinoína	16070001	1
Caelo	Tretinoína	16070002	2
Caelo	Tretinoína	16070003	1
Caelo	Tretinoína	1612010-01	4
Caelo	Tretinoína	1612010-02	2
Caelo	Tretinoína	16217107	1
Caelo	Tretinoína	16217108	3
Caelo	Tretinoína	16217112	2
Caelo	Tretinoína	16217120	1
Caelo	Tretinoína	16217122	3
Caelo	Tretinoína	16291502	6
Caelo	Tretinoína	16291503	8
Caelo	Tretinoína	16357602	1
Caelo	Tretinoína	16F14-B04	1
Caelo	Tretinoína	16F14-B04-324636	1
Caelo	Tretinoína	16F14-B04-326181	1
Caelo	Tretinoína	16K03-806328-388	1
Caelo	Tretinoína	17106101	4
Caelo	Tretinoína	17106102	15
Caelo	Tretinoína	171061025343	1
Caelo	Tretinoína	17106103	1
Caelo	Tretinoína	1723102	1
Caelo	Tretinoína	17273102	1
Caelo	Tretinoína	17273103	1
Caelo	Tretinoína	172773102	1
Caelo	Tretinoína	17305701	10
Caelo	Tretinoína	17305702	7
Caelo	Tretinoína	17305704	6
Caelo	Tretinoína	17305705	1
Caelo	Tretinoína	17305707	6
Caelo	Tretinoína	173057075597	1
Caelo	Tretinoína	17305708	1
Caelo	Tretinoína	17305709	2
Caelo	Tretinoína	17305710	2
Caelo	Tretinoína	17305711	1
Caelo	Tretinoína	17357001	11
Caelo	Tretinoína	17357002	7
Caelo	Tretinoína	17357004	1
Caelo	Tretinoína	17357005	2
Caelo	Tretinoína	17357007	7
Caelo	Tretinoína	17357008	4
Caelo	Tretinoína	17357009	5
Caelo	Tretinoína	1735707	1
Caelo	Tretinoína	17K01-B05-0005	1
Caelo	Tretinoína	17K01-B05-345784	1
Caelo	Tretinoína	1804005-01	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tretinoína	18167301	3
Caelo	Tretinoína	18167301P-190314-2	1
Caelo	Tretinoína	18167302	9
Caelo	Tretinoína	18167307	5
Caelo	Tretinoína	18167309	22
Caelo	Tretinoína	18167401	6
Caelo	Tretinoína	18167402	4
Caelo	Tretinoína	18167403	2
Caelo	Tretinoína	18167405	2
Caelo	Tretinoína	18167407	1
Caelo	Tretinoína	18167408	1
Caelo	Tretinoína	18167409	3
Caelo	Tretinoína	18167410	3
Caelo	Tretinoína	1901001-01	4
Caelo	Tretinoína	1903084002	1
Caelo	Tretinoína	190500003	1
Caelo	Tretinoína	19050001	13
Caelo	Tretinoína	19050003	18
Caelo	Tretinoína	1907014-01	1
Caelo	Tretinoína	1907014-02	1
Caelo	Tretinoína	191001-01	1
Caelo	Tretinoína	19185802	5
Caelo	Tretinoína	19185803	3
Caelo	Tretinoína	19185805	12
Caelo	Tretinoína	19185808	1
Caelo	Tretinoína	192571001	1
Caelo	Tretinoína	192571002	1
Caelo	Tretinoína	192571003	1
Caelo	Tretinoína	192571005	1
Caelo	Tretinoína	19257102	6
Caelo	Tretinoína	19257103	6
Caelo	Tretinoína	193084002	12
Caelo	Tretinoína	193084003	11
Caelo	Tretinoína	20000490001	5
Caelo	Tretinoína	20000490002	8
Caelo	Tretinoína	20000490005	5
Caelo	Tretinoína	20001881004	7
Caelo	Tretinoína	20004135001	7
Caelo	Tretinoína	20004135002	1
Caelo	Tretinoína	2004014-0	1
Caelo	Tretinoína	2004014-01	2
Caelo	Tretinoína	2004014-02	1
Caelo	Tretinoína	20120601	1
Caelo	Tretinoína	20A28-F01-368810	1
Caelo	Tretinoína	21000305002	8
Caelo	Tretinoína	21000305003	9
Caelo	Tretinoína	21000703001	7
Caelo	Tretinoína	21000703002	4
Caelo	Tretinoína	21000703004	3
Caelo	Tretinoína	21004211002	5
Caelo	Tretinoína	21004211003	12
Caelo	Tretinoína	21004211005	1
Caelo	Tretinoína	21004211007	3
Caelo	Tretinoína	2100421107	1
Caelo	Tretinoína	2205021-01	1
Caelo	Tretinoína	3041302	1
Caelo	Tretinoína	5012I-02563	1
Caelo	Tretinoína	711212563	1
Caeol/Noweda	Tretinoína	15437303	1
Caesar & Loretz /Gehe	Tretinoína	193084003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Tretinoína	21004211002	1
Caesar & Loretz GmbH...	Tretinoína	12023302	1
Caesar & Loretz GmbH...	Tretinoína	21004211005	1
Caesar & Loretz GmbH...	Tretinoína	193084003	1
Caesar & Loretz GmbH...	Tretinoína	19050001	1
Caesar & Loretz GmbH...	Tretinoína	20000490005	1
Caesar & Loretz GmbH/AHD	Tretinoína	19257103	1
Caesar & Loretz GmbH/AHD	Tretinoína	20000490002	1
Caesar & Loretz GmbH/AHD	Tretinoína	21000305002	1
Caesar & Loretz GmbH...	Tretinoína	19185802	1
Caesar & Loretz GmbH...	Tretinoína	20000490001	1
Caesar & Loretz GmbH...	Tretinoína	21000305002	2
Caesar & Loretz GmbH...	Tretinoína	193084002	1
Caesar & Loretz GmbH...	Tretinoína	19257103	2
Caesar & Loretz GmbH...	Tretinoína	193084002	1
Caesar & Loretz GmbH/gehe	Tretinoína	19257102	1
Caesar & Loretz GmbH/Gehe	Tretinoína	21000305003	1
Caesar & Loretz GmbH...	Tretinoína	21000703002	1
Caesar & Loretz GmbH...	Tretinoína	19185803	1
Caesar & Loretz GmbH...	Tretinoína	193084002	1
Caesar & Loretz GmbH...	Tretinoína	21000302002	1
Caesar & Loretz GmbH...	Tretinoína	21000305002	2
Caesar & Loretz GmbH/Sana	Tretinoína	193084003	1
Caesar & Loretz GmbH...	Tretinoína	21004211006	1
Caesar & Loretz GmbH...	Tretinoína	22002262001	1
Caesar & Loretz GmbH...	Tretinoína	193084002	1
Caesar & Loretz GmbH	Tretinoína	11225515	1
Caesar & Loretz GmbH	Tretinoína	12320211	1
Caesar & Loretz GmbH	Tretinoína	18167302	1
Caesar & Loretz GmbH	Tretinoína	18167309	1
Caesar & Loretz GmbH	Tretinoína	18167401	1
Caesar & Loretz GmbH	Tretinoína	18167408	1
Caesar & Loretz GmbH	Tretinoína	18167410	1
Caesar & Loretz GmbH	Tretinoína	19050001	2
Caesar & Loretz GmbH	Tretinoína	19050003	4
Caesar & Loretz GmbH	Tretinoína	19185801	1
Caesar & Loretz GmbH	Tretinoína	19185802	1
Caesar & Loretz GmbH	Tretinoína	19185803	2
Caesar & Loretz GmbH	Tretinoína	19185805	3
Caesar & Loretz GmbH	Tretinoína	192571001	1
Caesar & Loretz GmbH	Tretinoína	19257102	1
Caesar & Loretz GmbH	Tretinoína	19257103	4
Caesar & Loretz GmbH	Tretinoína	193084002	1
Caesar & Loretz GmbH	Tretinoína	193084003	6
Caesar & Loretz GmbH	Tretinoína	20000490001	2
Caesar & Loretz GmbH	Tretinoína	20000490002	4
Caesar & Loretz GmbH	Tretinoína	20000490005	1
Caesar & Loretz GmbH	Tretinoína	20001881004	2
Caesar & Loretz GmbH	Tretinoína	20001881005	1
Caesar & Loretz GmbH	Tretinoína	21000305001	1
Caesar & Loretz GmbH	Tretinoína	21000305002	1
Caesar & Loretz GmbH	Tretinoína	21000305003	9
Caesar & Loretz GmbH	Tretinoína	21000703001	5
Caesar & Loretz GmbH	Tretinoína	21000703004	1
Caesar & Loretz GmbH	Tretinoína	21004211002	2
Caesar & Loretz GmbH	Tretinoína	21004211003	2
Caesar & Loretz GmbH	Tretinoína	21004211005	3
Caesar & Loretz GmbH	Tretinoína	21004211007	1
Caesar & Loretz GmbH	Tretinoína	21004211009	1
Cealo/Phoenix	Tretinoína	19050003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
cealo	Tretinoína	13195002	1
Celo/Kehr	Tretinoína	16217122	1
Celo	Tretinoína	15437303	1
Eu Rho	Tretinoína	1612010-02	1
Eur Rho	Tretinoína	200401402	1
EuRho / AHD	Tretinoína	2106017-02	1
EuRho / Phoenix	Tretinoína	2205021-01	1
EuRho- Phoenix	Tretinoína	2106017-01	1
EURho/ Noweda	Tretinoína	1901001-01	1
EuRho/ Fiebig	Tretinoína	2004014-01	1
EuRho/ NOWEDA	Tretinoína	1804005-01	2
EuRho/ Noweda	Tretinoína	1907014-02	1
EuRho/ Sanacorp	Tretinoína	2205021-02	3
Eurho/Noweda	Tretinoína	2004014-02	1
EURho/Phoenix	Tretinoína	1907014-01	1
Eurho/Phönix	Tretinoína	2205021	1
EuRho/Sanacorp	Tretinoína	130402802	1
EuRho/Sanacorp	Tretinoína	210601703	1
EuRho/Spangro	Tretinoína	1901001-01	1
EuRho	Tretinoína	151007-01	1
EuRho	Tretinoína	1804005-01	1
EuRho	Tretinoína	19042068	1
EuRho	Tretinoína	1907014-01	1
EuRho	Tretinoína	190701402	1
EuRho	Tretinoína	1907014-02	1
EuRho	Tretinoína	2004014-02	4
EuRho	Tretinoína	2205021-01	1
Eurimpharm	Tretinoína	1411016-01	1
Euro OCT Pharma/Fiebig	Tretinoína	1604059-01	2
Euro OT/ Gehe	Tretinoína	1901001-01	2
Euro OTC	Tretinoína	1008021-02	1
Euro OTC	Tretinoína	10429AX21	1
Euro OTC	Tretinoína	1109014-02	2
Euro OTC	Tretinoína	12059AX20	2
Euro OTC	Tretinoína	12959AX20	3
Euro OTC	Tretinoína	130102802	1
Euro OTC	Tretinoína	1304028-01	7
Euro OTC	Tretinoína	130402802	1
Euro OTC	Tretinoína	1304028-02	6
Euro OTC	Tretinoína	13041028-01	1
Euro OTC	Tretinoína	140007-02	1
Euro OTC	Tretinoína	14020007-01	1
Euro OTC	Tretinoína	1402007	1
Euro OTC	Tretinoína	140200701	1
Euro OTC	Tretinoína	1402007-01	5
Euro OTC	Tretinoína	1402007-02	9
Euro OTC	Tretinoína	140200703	1
Euro OTC	Tretinoína	1402007-03	3
Euro OTC	Tretinoína	14101602	1
Euro OTC	Tretinoína	1411016-01	12
Euro OTC	Tretinoína	141101602	1
Euro OTC	Tretinoína	1411016-02	12
Euro OTC	Tretinoína	141107602	1
Euro OTC	Tretinoína	151000	1
Euro OTC	Tretinoína	1510007-01	13
Euro OTC	Tretinoína	151000702	1
Euro OTC	Tretinoína	1510007-02	17
Euro OTC	Tretinoína	16004059-02	1
Euro OTC	Tretinoína	160405901	1
Euro OTC	Tretinoína	1604059-01	23

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tretinoína	160405902	2
Euro OTC	Tretinoína	1604059-02	21
Euro OTC	Tretinoína	16052905	1
Euro OTC	Tretinoína	161201001	2
Euro OTC	Tretinoína	1612010-01	30
Euro OTC	Tretinoína	1612010-02	15
Euro OTC	Tretinoína	161210-01	1
Euro OTC	Tretinoína	162010-02	1
Euro OTC	Tretinoína	16217108	1
Euro OTC	Tretinoína	165070002	1
Euro OTC	Tretinoína	17273103	1
Euro OTC	Tretinoína	17357001	2
Euro OTC	Tretinoína	17Ko1-Bo5-345784	1
Euro OTC	Tretinoína	180400501	4
Euro OTC	Tretinoína	1804005-01	49
Euro OTC	Tretinoína	1804008-01	1
Euro OTC	Tretinoína	18062082	2
Euro OTC	Tretinoína	18167302	1
Euro OTC	Tretinoína	18167405	1
Euro OTC	Tretinoína	184005-01	1
Euro OTC	Tretinoína	18432003	3
Euro OTC	Tretinoína	18J30-B02-359836	1
Euro OTC	Tretinoína	190100-01	1
Euro OTC	Tretinoína	190100101	2
Euro OTC	Tretinoína	1901001-01	44
Euro OTC	Tretinoína	190100102	1
Euro OTC	Tretinoína	1901001-02	20
Euro OTC	Tretinoína	19042068	3
Euro OTC	Tretinoína	19042092	3
Euro OTC	Tretinoína	1907014	1
Euro OTC	Tretinoína	190701401	4
Euro OTC	Tretinoína	1907014-01	22
Euro OTC	Tretinoína	190701402	1
Euro OTC	Tretinoína	1907014-02	42
Euro OTC	Tretinoína	190714-02	2
Euro OTC	Tretinoína	2001014-01	1
Euro OTC	Tretinoína	2001014-02	2
Euro OTC	Tretinoína	2004014	2
Euro OTC	Tretinoína	2004014-01	45
Euro OTC	Tretinoína	2004014-02	41
Euro OTC	Tretinoína	20332110	1
Euro OTC	Tretinoína	2105017-01	1
Euro OTC	Tretinoína	2106017	1
Euro OTC	Tretinoína	2106017_03	1
Euro OTC	Tretinoína	210601701	2
Euro OTC	Tretinoína	2106017-01	15
Euro OTC	Tretinoína	2106017-02	24
Euro OTC	Tretinoína	2106017-03	11
Euro OTC	Tretinoína	2205021-01	11
Euro OTC	Tretinoína	230301701	1
Euro OTC	Tretinoína	2303017-01	2
Euro OTC	Tretinoína	2994014-02	1
Euro OTC	Tretinoína	30042014A	1
Euro OTC	Tretinoína	5219Q-02563	1
Euro OTC	Tretinoína	67(1804005-01)	1
Euro OTC	Tretinoína	819081-16	1
Euro OTC	Tretinoína	99999999	1
Euro/Gehe	Tretinoína	1604059-01	1
Euro/Noweda	Tretinoína	1612010-01	1
Euro/Phoenix	Tretinoína	1901001-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Phoenix	Tretinoína	1907014-01	1
Euro/Phönix	Tretinoína	18J30B02359836	1
Euro/Phönix	Tretinoína	1907014-01	1
Euro/Sanacorp	Tretinoína	1604059-02	1
Euro	Tretinoína	14111016-01	1
Euroo/Phönix	Tretinoína	210601703	1
EuroPharm/ Sanacorp	Tretinoína	1804005-01	1
Fagron	Tretinoína	11K29-N01	1
Fagron	Tretinoína	12I06-N01	2
Fagron	Tretinoína	12106-N01	1
Fagron	Tretinoína	13B05-B02-287360	4
Fagron	Tretinoína	13B05-B02-287361	2
Fagron	Tretinoína	13C11-N06	2
Fagron	Tretinoína	13D30N14	1
Fagron	Tretinoína	13D30-N14	2
Fagron	Tretinoína	13D30-N14-3365319091	1
Fagron	Tretinoína	14009-804	1
Fagron	Tretinoína	14040504	1
Fagron	Tretinoína	14093505	1
Fagron	Tretinoína	1410001594	1
Fagron	Tretinoína	1411016-01	1
Fagron	Tretinoína	1440104	1
Fagron	Tretinoína	14D09-B04	1
Fagron	Tretinoína	14D09-B04-293224	1
Fagron	Tretinoína	14D09-B04-293225	1
Fagron	Tretinoína	14D09-B04-293594	1
Fagron	Tretinoína	14D09-B04-295551	1
Fagron	Tretinoína	14L24-B01	1
Fagron	Tretinoína	14L24-B01-303152	1
Fagron	Tretinoína	14L24-B01-303157	4
Fagron	Tretinoína	1510007-01	1
Fagron	Tretinoína	1510007-02	1
Fagron	Tretinoína	15F01-B06-308722	7
Fagron	Tretinoína	15F01-B06-308856	4
Fagron	Tretinoína	15F01-B06-313216	2
Fagron	Tretinoína	15F01-B06-315491	1
Fagron	Tretinoína	15F01-B06-317884	1
Fagron	Tretinoína	1604059-01	1
Fagron	Tretinoína	16052905	4
Fagron	Tretinoína	16F14-B04	3
Fagron	Tretinoína	16F14-B04-324636	2
Fagron	Tretinoína	16f14-b04-325560	1
Fagron	Tretinoína	16F14B04325560	1
Fagron	Tretinoína	16F14-B04-325560	2
Fagron	Tretinoína	16F-14-B04-325560	1
Fagron	Tretinoína	16F14-B04-325567	1
Fagron	Tretinoína	16F14-B04-326181	2
Fagron	Tretinoína	16F14B04325560	1
Fagron	Tretinoína	16K03-B06	3
Fagron	Tretinoína	16K03-B06-328388	5
Fagron	Tretinoína	170706TTRER-20151004	1
Fagron	Tretinoína	17273102	1
Fagron	Tretinoína	17357007	1
Fagron	Tretinoína	17K01-B05	2
Fagron	Tretinoína	17K01-B05-341936	8
Fagron	Tretinoína	17K01-B05-341941	2
Fagron	Tretinoína	17K01-B05-345784	4
Fagron	Tretinoína	17K01-B05-347435	3
Fagron	Tretinoína	17K01-B05-347436	1
Fagron	Tretinoína	17K01B05349946	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tretinoína	17K01-B05-349946	4
Fagron	Tretinoína	18167404	1
Fagron	Tretinoína	18A10-B03-344364	1
Fagron	Tretinoína	18J30-B02	2
Fagron	Tretinoína	18J30-B02_359836	1
Fagron	Tretinoína	18j30B02358540	1
Fagron	Tretinoína	18J30-B02-358540	4
Fagron	Tretinoína	18J30-B02-358546	1
Fagron	Tretinoína	18J30-B02-358547	1
Fagron	Tretinoína	18J30-B02-359836	1
Fagron	Tretinoína	18J30-B02-362110	5
Fagron	Tretinoína	18J30-B02-362120	1
Fagron	Tretinoína	19K07-06-366648	1
Fagron	Tretinoína	19K07-F06	4
Fagron	Tretinoína	19K07-F06-366648	12
Fagron	Tretinoína	20000490002	2
Fagron	Tretinoína	20110004	1
Fagron	Tretinoína	20120601	1
Fagron	Tretinoína	20A28-F01-368810	2
Fagron	Tretinoína	20A28-F01-368813	1
Fagron	Tretinoína	21E17-F03-378623	2
Fagron	Tretinoína	21G10-B08	1
Fagron	Tretinoína	21G10-B08-213327	2
Fagron	Tretinoína	22080001	1
Fagron	Tretinoína	231115T	1
Fagron	Tretinoína	23A23-B12-225240	1
Fagron	Tretinoína	6366648	1
Fagron	Tretinoína	F01-3688100	2
Fagron	Tretinoína	TRER-20180703	2
Fargon	Tretinoína	16K03-B06-328388	1
Fargron/ Sanacorp	Tretinoína	17k01-b05-341936	1
Fargron	Tretinoína	1402007-01	1
Fargron	Tretinoína	14D09-B04-293225	1
FEJ	Tretinoína	15F01-B06-308856	1
Fiebig	Tretinoína	1612010-01	1
Gatt-Koller	Tretinoína	1702180	1
Gatt-Koller	Tretinoína	1804193	1
Gatt-Koller	Tretinoína	606210909	1
Gehe am 11.10.2017	Tretinoína	17106102	1
Gehe amax	Tretinoína	1604059-02	1
Gehe	Tretinoína	15078307	1
Gehe	Tretinoína	1510007-01	1
Gehe	Tretinoína	15437303	1
Gehe	Tretinoína	1604059-02	1
Gehe	Tretinoína	1612010-01	1
Gehe	Tretinoína	1901001-01	1
Gehe	Tretinoína	1901001-02	1
Gehe	Tretinoína	19050001	1
GEHE	Tretinoína	19050001	1
Gehe	Tretinoína	1907014-01	2
Gehe	Tretinoína	1907014-02	1
Gehe	Tretinoína	2106017-01	1
Gehe	Tretinoína	2205021-02	1
GEHE	Tretinoína	2205021-02	1
Gehe-Eurho 22.11.2017	Tretinoína	2171127Ma7	1
Geibo	Tretinoína	17K01-B05-341936	1
JENNE	Tretinoína	17K01-B05-341941	1
Jenne	Tretinoína	1901001-01	1
Kehr	Tretinoína	1604059-01	1
Krieger am 17.08.2018	Tretinoína	17K01-B05-345784	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Krieger	Tretinoína	1612010-02	2
Krieger	Tretinoína	2205021-02	1
L10	Tretinoína	1612010-01	2
Nachprüfung	Tretinoína		1
Nachprüfung	Tretinoína	2605001-01	1
Noweda/EuRho 06.05.2...	Tretinoína	2004014-01	1
Noweda/EuRho	Tretinoína	2106017-02	1
Noweda	Tretinoína	12023302	2
Noweda	Tretinoína	13D30-N14	1
Noweda	Tretinoína	15078307	1
Noweda	Tretinoína	15F01-B06-315491	1
Noweda	Tretinoína	17305701	1
Noweda	Tretinoína	1804005-01	3
Noweda	Tretinoína	18167402	1
Noweda	Tretinoína	19257103	1
Noweda	Tretinoína	200401402	1
Noweda	Tretinoína	2004014-02	1
Noweda	Tretinoína	2205021-01	2
Noweda	Tretinoína	2205021-02	1
Phoenix	Tretinoína	12367103	1
Phoenix	Tretinoína	15F01-B06-317884	1
Phoenix	Tretinoína	190701402	1
Phoenix	Tretinoína	19K07-F06-366648	1
Phoenix	Tretinoína	200401401	3
Phoenix	Tretinoína	2004014-01	3
Phoenix	Tretinoína	2106017-03	1
Phoenix	Tretinoína	2205021-02	1
Phönix WE:04.01.18 ...	Tretinoína	17273102	1
Phönix	Tretinoína	1109014-02	1
Phönix	Tretinoína	1402007-02	1
Phönix	Tretinoína	14D09-B04	2
Phönix	Tretinoína	14D09-B04-293224	1
phönix	Tretinoína	1612010-01	1
phönix	Tretinoína	17273102	1
Phönix	Tretinoína	17k01-b05-349946	1
Phönix	Tretinoína	18167302	1
Phönix	Tretinoína	1901001-01	1
Phönix	Tretinoína	200831409	1
Phönix	Tretinoína	200931709	1
Phönix	Tretinoína	2205021-01	1
Phönix	Tretinoína	3144	1
Sana	Tretinoína	21G10-B08-213327	1
Sanacorp/EuRho	Tretinoína	1604059-02	1
Sanacorp	Tretinoína	12/06-N01	1
Sanacorp	Tretinoína	12320302	1
Sanacorp	Tretinoína	13308004	1
Sanacorp	Tretinoína	1411016-01	1
Sanacorp	Tretinoína	1411016-02	1
Sanacorp	Tretinoína	14L24-B01	1
Sanacorp	Tretinoína	16217122	1
Sanacorp	Tretinoína	17357001	1
Sanacorp	Tretinoína	1804005-01	1
Sanacorp	Tretinoína	18167309	1
Sanacorp	Tretinoína	1907014-02	1
Sanacorp	Tretinoína	19185805	1
Sanacorp	Tretinoína	193084003	1
Sanacorp	Tretinoína	21000305001	1
Sanacorp	Tretinoína	2205021-01	1
Sanacorp	Tretinoína	2303017-01	1
Sanacorp	Tretinoína	2311013-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Siegfried Chemikalie…	Tretinoína	1804005	1
Siegfried Pharamchikalien	Tretinoína	2004014-01	1
Siegfried Pharm. Che…	Tretinoína	17K01-B05-345784	1
Siegfried Pharma / Gehe	Tretinoína	1907014-01	1
Siegfried Pharma / Gehe	Tretinoína	1907014-02	1
siegfried pharma che…	Tretinoína	2106017-01	1
Siegfried PharmaChem…	Tretinoína	1907014-02	1
Siegfried Pharmachem…	Tretinoína	2004014-01	1
Siegfried Pharmachem…	Tretinoína	19042092	1
Siegfried Pharmachem…	Tretinoína	2004014-01	1
Siegfried Pharmachem…	Tretinoína	2004014-02	1
Siegfried PharmaChem…	Tretinoína	18432003	1
Siegfried PharmaChem…	Tretinoína	19042092	1
Synthetisch/GEIBO	Tretinoína	2106017-03	1
synthetisch	Tretinoína	2106017-02	1
WE:Phönix 20.08.201…	Tretinoína	1510007-02	1
WE:Phönix 02.11..201…	Tretinoína	1604059-01	1

- 234 418 spectra from 1515 *Apo-Ident* customers from a total of 48 925 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tretinoína* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tretinoína* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	600	0	152 362
Type B	0	1460	0	200 624
Type C	0	1569	80	234 418

The substance/substance group *Tretinoína* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5890 %)
Type C	100.0000 % (> 99.9007 %)	95.1486 % (> 94.9666 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21747	21747	0,00	128,52
21757	21757	0,00	105,87
21878	21747	21,99	120,80
21940	21940	0,00	119,65
22574	22574	0,00	109,65
22936	21940	7,04	113,46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triancinolona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20564-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triancinolona; Triamcinolonum

Special notes

When selecting the *Triancinolona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triancinolona	9	3	58

Second-stage model

For differentiation of the substance/substance group *Triancinolona* the following second-stage model is used:

- Submodelo 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triancinolona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato sódico de riboflavina hidratado	66,53	–
⋮	⋮	⋮
Cianocobalamina	>50	36,47
Sulfato de polimixina B	67,00	38,25
Bacitracina	>50	42,86
Anfotericina B	>50	50,61
Sulfato de colistina	>50	56,25
Riboflavina	>50	56,97
Metilcobalamina	>50	62,62
Pantotenato de cálcio	>50	67,49
Nistatina	>50	85,37
Estradiol hemi-hidratado	>50	90,28
Estriol	>50	95,20
Bromidrato de hioscina	>50	103,27
Tosilcloramida sódica	>50	114,53
Gelatina, branca	>50	115,38
Vitamina E acetato pó 50%	>50	147,74
Glicerofosfato de cálcio	>50	150,96
Levedura de selênio	>50	187,33
SyrSpend® SF pH4 neo	>50	187,44
SyrSpend® SF Alka	>50	202,10
Ácido oxálico	>50	223,18
Amido de arroz	>50	248,31
Carmelose sódica	>50	254,47
Amido de milho	>50	339,13
SyrSpend® SF pH4	>50	348,51
Goma arábica, dispersão seca	>50	392,17
Amido de trigo	>50	409,92
Maltodextrina	>50	462,17
Fécula de batata	>50	464,46
Frutose	>50	469,05

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triancinolona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triancinolona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triancinolona	15106905	22273	45	20150527
Caelo	Triancinolona	15106905	22605	40	20150527
Caelo	Triancinolona	20001706	25555	40	20200902*
Caelo	Triancinolona	20001706	25555SI	35	20200902*
Fagron	Triancinolona	12A03-N09	20730	40	20120117
Fagron	Triancinolona	12K07-N13	20936	80	AR-15-FG-003373-01
Fagron	Triancinolona	14B13-B30-316101	22840	40	20140311
Fagron	Triancinolona	18A19-B05-351174	24182	40	1811263
Fagron	Triancinolona	18A19-B05-351174	24182SI	32	1811263
Fagron	Triancinolona	18E09-B04-353921	24446	40	1907730
Fagron	Triancinolona	18J01-B05-364078	24944	40	2004435
Fagron	Triancinolona	22A17-B05-216480	26140	40	20220421

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 512 spectra of 12 reference samples from the substance/substance group *Triancinolona*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.
- 152 450 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 10 reference samples from the substance/substance group *Triancinolona*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triancinolona	15106911	23508	40
Fagron	Triancinolona	17G03-B04-343670	24097	40
Fagron	Triancinolona	21H13-B19-215838	25938	40
Fagron	Triancinolona	17G03-B04-343670	24097SI	40
Fagron	Triancinolona	17G03-B04-343670	24107	40
Fagron	Triancinolona	17G03-B04-343670	24107SI	40
Fagron	Triancinolona	18E09-B04-353921	24446SI†	40
Fagron	Triancinolona	18J01-B05-364078	24944SI†	40
Fagron	Triancinolona	21H13-B19-215838	25938SI	40
Fagron	Triancinolona	22A17-B05-216480	26140SI†	40

- 201 684 spectra from a total of 4039 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 95 spectra from 58 *Apo-Ident* customers from 62 batches from the substance/substance group *Triancinolona*.

- Among them are spectra of independent samples from 58 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Triancinolona	22A17-B05-222384	1
	Triancinolona	22J05B05227276	1
	Triancinolona	22J05-B05-227276	2
Caelo	Triancinolona	12295207	3
Caelo	Triancinolona	12295210	1
Caelo	Triancinolona	13J07-N08	2
Caelo	Triancinolona	14B13-B30-293474	1
Caelo	Triancinolona	14B13-B30312868	1
Caelo	Triancinolona	15106902	1
Caelo	Triancinolona	15106912	1
Caelo	Triancinolona	15106960	1
Caelo	Triancinolona	180921002	3
Caelo	Triancinolona	18092104	3
Caesar & Loretz GmbH...	Triancinolona	21001467001	1
Caesar & Loretz GmbH	Triancinolona	21001467001	1
Fagron	Triancinolona	11D28-N04	1
Fagron	Triancinolona	11G26-N04	1
Fagron	Triancinolona	12A03-N09	1
Fagron	Triancinolona	12D02-N14	1
Fagron	Triancinolona	12Do2-N14	1
Fagron	Triancinolona	12F01-N19	3
Fagron	Triancinolona	13C26-N04	1
Fagron	Triancinolona	13D30-N15	2
Fagron	Triancinolona	13J07-N08	1
Fagron	Triancinolona	14A14-B01	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triancinolona	14B13-B30	1
Fagron	Triancinolona	14B13-B30-293473	1
Fagron	Triancinolona	14B13-B30-312868	1
Fagron	Triancinolona	14B13-B30-316102	1
Fagron	Triancinolona	15B13-B30-312868	1
Fagron	Triancinolona	16A13-B06	2
Fagron	Triancinolona	18A19-B05-352984	3
Fagron	Triancinolona	18E09-B04-355656	1
Fagron	Triancinolona	18J01-B05	2
Fagron	Triancinolona	18J01-B05-364078	2
Fagron	Triancinolona	18J01B05364080	1
Fagron	Triancinolona	18J01-B05-364080	1
Fagron	Triancinolona	20k25-f03	1
Fagron	Triancinolona	20K25-F03	2
Fagron	Triancinolona	20K25-F03-376111	2
Fagron	Triancinolona	20K25-F03-376112	4
Fagron	Triancinolona	20K25-F03-377107	1
Fagron	Triancinolona	21I03-B01-216482	1
Fagron	Triancinolona	21l03-B01_216482	1
Fagron	Triancinolona	21l03-B01-216482	1
Fagron	Triancinolona	22A17-B05	1
Fagron	Triancinolona	22A17-B05-216480	3
Fagron	Triancinolona	F03-3761102	1
Fagron	Triancinolona	NT1484M	1
Fagron	Triancinolona	NTL171102	1
Fagron	Triancinolona	NTL200702	2
Fargon/Gehe	Triancinolona	B04-3539201	1
Fargon/Gehe	Triancinolona	B05-3640708	1
Fargon	Triancinolona	18J01-B05-364078	1
Gehe	Triancinolona	16F07-B01-331398	1
Gehe	Triancinolona	NTL180603	1
L12	Triancinolona	17359001	1
Noweda 24.08.2015	Triancinolona	14B13-B30-293474	1
Noweda	Triancinolona	21/03-B01-216482	2
Noweda	Triancinolona	22A17-B05-222384	1
Noweda	Triancinolona	22J05-B05-227276	1
Phönix	Triancinolona	18A19B05-352890	1
Phönix	Triancinolona	NS0608M	1
Sanacorp	Triancinolona	100/AKD6	1
Sanacorp	Triancinolona	15106907	1
Sanacorp	Triancinolona	15106916	1
Sanacorp	Triancinolona	23F26-B02-229454	2
Tianjin Tianyao Phar…	Triancinolona	18J01-B05-364080	1
Tianjin Tianyao Phar…	Triancinolona	21I03-B01-216482	1

- 235 972 spectra from 1515 *Apo-Ident* customers from a total of 49 197 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triancinolona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triancinolona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	512	0	152 450
Type B	0	384	16	201 684
Type C	0	88	7	235 972

The substance/substance group *Triancinolona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8281 %)
Type B	100.0000 % (> 99.9912 %)	96.0000 % (> 95.2500 %)
Type C	100.0000 % (> 99.9007 %)	92.6316 % (> 89.4737 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20730	20936	50,54	150,17
20936	20936	0,00	183,24
22273	25555	12,72	184,88
22605	25555	9,37	179,99
22840	25555	12,40	178,74
24182	24182	0,00	112,46
24446	24446	0,00	124,59
24944	24944	0,00	103,03
25555	25555	0,00	181,88
26140	24182	42,93	109,47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triancinolona acetonido**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20765-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triancinolona acetonido; Triamcinoloni acetonidum

Special notes

When selecting the *Triancinolona acetonido* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triancinolona acetonido	12	24	810

Second-stage model

For differentiation of the substance/substance group *Triancinolona acetonido* the following second-stage model is used:

- Submodelo 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triancinolona acetonido* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	63,83	–
⋮	⋮	⋮
Fluocinolona acetonida	73,86	34,92
Prednisolona	>50	61,12
Betametasona	>50	63,08
Metilprednisolona	>50	77,88
Tirotricina	>50	90,87
Dexametasona	>50	96,52
Gramicidina	>50	136,76

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triancinolona acetonido* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triancinolona acetonido*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triancinolona acetonido	13256607	21061	100	AR-15-FG-003755-01
Caelo	Triancinolona acetonido	13379921	21587	60	1503634
Caelo	Triancinolona acetonido	20002630	25560	40	20200902*
Caelo	Triancinolona acetonido	20002630	25560SI	31	20200902*
Euro OTC	Triancinolona acetonido	1303001-02	20910	40	20130815
Euro OTC	Triancinolona acetonido	1211013-02	21072	30	20130417
Euro OTC	Triancinolona acetonido	1508008	21883	60	20150902*
Euro OTC	Triancinolona acetonido	1601021	22313	45	20160119*
Euro OTC	Triancinolona acetonido	1605010	22572	40	20160531*
Euro OTC	Triancinolona acetonido	1605010	22572SI	25	20160531*
Euro OTC	Triancinolona acetonido	1608005	22752	40	20160906*
Euro OTC	Triancinolona acetonido	1608005	22752SI	22	20160906*
Euro OTC	Triancinolona acetonido	2006002	25339	40	2011401

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triancinolona acetonido	2006002	25339SI	29	2011401
Fagron	Triancinolona acetonido	12E15-N03	20765	60	1412051
Fagron	Triancinolona acetonido	15C19-B06-308572	21962	60	20150402

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 722 spectra of 16 reference samples from the substance/substance group *Triancinolona acetonido*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 240 spectra from a total of 2830 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1679 spectra of 50 reference samples from the substance/substance group *Triancinolona acetonido*.

- Among them are spectra of independent samples from 24 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triancinolona acetonido	12301505	20769	60
Caelo	Triancinolona acetonido	160945	22473	60
Caelo	Triancinolona acetonido	171206	23330	40
Caelo	Triancinolona acetonido	181002	24016	40
Caelo	Triancinolona acetonido	190619	24509	40
Caelo	Triancinolona acetonido	23002617	26965	40
Euro OTC	Triancinolona acetonido	1612014	22978	40
Euro OTC	Triancinolona acetonido	1703037	23393	40
Euro OTC	Triancinolona acetonido	1706013	23557	40
Euro OTC	Triancinolona acetonido	1710002	23694	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Triancinolona acetonido	1801020	23883	40
Euro OTC	Triancinolona acetonido	1805001-01	24191	40
Euro OTC	Triancinolona acetonido	1810015	24333	40
Euro OTC	Triancinolona acetonido	1903015	24629	40
Euro OTC	Triancinolona acetonido	1907044	24842	40
Euro OTC	Triancinolona acetonido	2001017	25115	40
Euro OTC	Triancinolona acetonido	2002047	25117	40
Euro OTC	Triancinolona acetonido	2006032	25456	40
Euro OTC	Triancinolona acetonido	2012006	25526	40
Euro OTC	Triancinolona acetonido	2109004	25832	50
Euro OTC	Triancinolona acetonido	2208004	26261	40
Euro OTC	Triancinolona acetonido	2308018	26930	40
Fagron	Triancinolona acetonido	13C13-N20	21043	60
Fagron	Triancinolona acetonido	22A22-B02-221452	26131	40
Caelo	Triancinolona acetonido	160945	22473SI	40
Caelo	Triancinolona acetonido	171206	23330SI	20
Caelo	Triancinolona acetonido	171206	23343	40
Caelo	Triancinolona acetonido	171206	23343SI	20
Caelo	Triancinolona acetonido	181002	24016SI	20
Caelo	Triancinolona acetonido	190619	24509SI	20
Caelo	Triancinolona acetonido	23002617	26965SI	30
Euro OTC	Triancinolona acetonido	1508008	21883SI[†]	30
Euro OTC	Triancinolona acetonido	1612014	22978SI	29
Euro OTC	Triancinolona acetonido	1703037	23393SI	20
Euro OTC	Triancinolona acetonido	1706013	23557SI	20
Euro OTC	Triancinolona acetonido	1710002	23694SI	20
Euro OTC	Triancinolona acetonido	1801020	23883SI	20
Euro OTC	Triancinolona acetonido	1805001-01	24191SI	20
Euro OTC	Triancinolona acetonido	1810015	24333SI	20
Euro OTC	Triancinolona acetonido	1903015	24629SI	20
Euro OTC	Triancinolona acetonido	1907044	24842SI	20
Euro OTC	Triancinolona acetonido	2001017	25115SI	40
Euro OTC	Triancinolona acetonido	2002047	25117SI	20
Euro OTC	Triancinolona acetonido	2006032	25456SI	20
Euro OTC	Triancinolona acetonido	2012006	25526SI	20
Euro OTC	Triancinolona acetonido	2109004	25832SI	30
Euro OTC	Triancinolona acetonido	2208004	26261SI	30
Euro OTC	Triancinolona acetonido	2308018	26930SI	31
Fagron	Triancinolona acetonido	15C19-B06-308572	21962SI[†]	19
Fagron	Triancinolona acetonido	22A22-B02-221452	26131SI	30

- 200 405 spectra from a total of 4019 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5559 spectra from 1283 *Apo-Ident* customers from 846 batches from the substance/substance group *Triancinolona acetonido*.

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- Among them are spectra of independent samples from 807 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Triancinolona acetonido	1403009-01	1
	Triancinolona acetonido	2012006-01	1
	Triancinolona acetonido	21000116011	1
	Triancinolona acetonido	21003093011	1
	Triancinolona acetonido	21003093012	1
	Triancinolona acetonido	21003093013	3
	Triancinolona acetonido	2109004-01	2
	Triancinolona acetonido	2109004-03	2
	Triancinolona acetonido	21H25-F03-379863	1
	Triancinolona acetonido	21H25-F03-379875	1
	Triancinolona acetonido	2200004-01	1
	Triancinolona acetonido	220000902012	1
	Triancinolona acetonido	22000902001	3
	Triancinolona acetonido	22000902002	3
	Triancinolona acetonido	22000902004	1
	Triancinolona acetonido	22000902005	4
	Triancinolona acetonido	22000902008	7
	Triancinolona acetonido	22000902009	10
	Triancinolona acetonido	22000902010	6
	Triancinolona acetonido	22000902012	3
	Triancinolona acetonido	22000902013	1
	Triancinolona acetonido	22000902014	2
	Triancinolona acetonido	22000902015	1
	Triancinolona acetonido	22000902016	8
	Triancinolona acetonido	22000902018	7
	Triancinolona acetonido	22000902019	5
	Triancinolona acetonido	2200090212	1
	Triancinolona acetonido	2208004-01	34
	Triancinolona acetonido	2208004-02	6
	Triancinolona acetonido	22A22-B01-218005	2
	Triancinolona acetonido	22A2-B01-218005	1
	Triancinolona acetonido	22D15-B01-220144	2
	Triancinolona acetonido	22D15-B01-222391	2
	Triancinolona acetonido	22D15-B01-222393	2
	Triancinolona acetonido	23002018-02	1
	Triancinolona acetonido	23002073005	1
	Triancinolona acetonido	23003235001	1
	Triancinolona acetonido	2305018-01	1
	Triancinolona acetonido	2308018-01	6
	Triancinolona acetonido	2308018-02	1
	Triancinolona acetonido	23C28-B04-227509	1
	Triancinolona acetonido	NB0601M	2
16804-B07	Triancinolona acetonido	16B04/B07	1
2001017-0	Triancinolona acetonido	2001017-01	1
A.H. 07.05.13 ek: 7,25EUR	Triancinolona acetonido	1211013-02	1
A.H.D.	Triancinolona acetonido	12301508	1
AHD 03.03.2015	Triancinolona acetonido	NT1430M	1
AHD 06.03.15 9,47	Triancinolona acetonido	14355102	2
AHD 17.07.2020	Triancinolona acetonido	NA0088M	1
AHD 22.12.16 EK 29,74	Triancinolona acetonido	16D14B11322136	1
AHD/Hedinger	Triancinolona acetonido	15233902	1
AHD	Triancinolona acetonido	14355711	1
AHD	Triancinolona acetonido	17057905	4
AHD	Triancinolona acetonido	20B28-F04-371546	1
AHD	Triancinolona acetonido	21003093001	1
AHD	Triancinolona acetonido	22000902009	1
AHD	Triancinolona acetonido	22000902018	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Triancinolona acetonido	22000902019	1
AHD	Triancinolona acetonido	2208004-01	2
AHD	Triancinolona acetonido	2208004-02	1
AHD	Triancinolona acetonido	APU0544/315240T	1
AhHD	Triancinolona acetonido	22000902016	1
Alliance Healthcare	Triancinolona acetonido	13C13-N20	2
Alliance Healthcare	Triancinolona acetonido	21000116001	1
Alliance	Triancinolona acetonido	21003093001	1
Alliance	Triancinolona acetonido	22000902009	1
Alliance	Triancinolona acetonido	2208004-01	2
Allianz Healthcare	Triancinolona acetonido	16080005-01	1
almirall/gehe	Triancinolona acetonido	17120607	4
Anzag	Triancinolona acetonido	1303001-02	1
Anzag	Triancinolona acetonido	14355103	1
Anzag	Triancinolona acetonido	14355711	1
Anzag	Triancinolona acetonido	1605010-01	1
Anzag	Triancinolona acetonido	17120605	1
Anzag	Triancinolona acetonido	20002630005	1
Anzag	Triancinolona acetonido	201200601	1
Anzag	Triancinolona acetonido	2012006-01	1
Anzag	Triancinolona acetonido	2208004-01	1
apo ident	Triancinolona acetonido	1612014-01	1
Apo Ident	Triancinolona acetonido	1907044-01	1
APO III	Triancinolona acetonido	21003093005	1
apoident	Triancinolona acetonido	1508008-01	1
apo-ident	Triancinolona acetonido	1608005-01	1
apo-ident	Triancinolona acetonido	1801020-01	1
apo-ident	Triancinolona acetonido	1810015-01	1
apomix	Triancinolona acetonido	13k15-b31-289029	2
apomix	Triancinolona acetonido	17120606	2
Apotheke Mildenau	Triancinolona acetonido	13C13-N20	1
Audor Pharma	Triancinolona acetonido	15240T	1
Audor Pharma	Triancinolona acetonido	APNET180403T	3
Audor Pharma	Triancinolona acetonido	APU0544/315240T	3
Audor Pharma	Triancinolona acetonido	APU0544/3162705	1
Audor Pharma	Triancinolona acetonido	APU0544/316270T	2
Audor Pharma	Triancinolona acetonido	APU0544/317171T	1
Audor Pharma	Triancinolona acetonido	APU0544/31524T	1
Audor Pharma	Triancinolona acetonido	U0544/315240T	1
Beiersdorf	Triancinolona acetonido	18F14-B01-351889	1
Berkel AHK	Triancinolona acetonido	14355101	3
Bombas/Sanac	Triancinolona acetonido	16094506	1
Bombastus	Triancinolona acetonido	13K15-B31	2
Bombastus	Triancinolona acetonido	17120610	1
Bombastus	Triancinolona acetonido	1810015-01	1
Cael/Sanacorp	Triancinolona acetonido	171002-01	1
Caelo	Triancinolona acetonido	100/AKD2	1
Caelo	Triancinolona acetonido	10220341	1
Caelo	Triancinolona acetonido	1040417	1
Caelo	Triancinolona acetonido	11022021-02	1
Caelo	Triancinolona acetonido	1107212516	1
Caelo	Triancinolona acetonido	1110005-01	1
Caelo	Triancinolona acetonido	1120717/16094502	1
Caelo	Triancinolona acetonido	11267704	1
Caelo	Triancinolona acetonido	11267705	1
Caelo	Triancinolona acetonido	11267707	4
Caelo	Triancinolona acetonido	11267710	2
Caelo	Triancinolona acetonido	11267720	1
Caelo	Triancinolona acetonido	11267721	2
Caelo	Triancinolona acetonido	116D14B11325479	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triancinolona acetonido	12/10-N09	3
Caelo	Triancinolona acetonido	1201506	1
Caelo	Triancinolona acetonido	12031601	1
Caelo	Triancinolona acetonido	1206008-01	1
Caelo	Triancinolona acetonido	1209040-01	1
Caelo	Triancinolona acetonido	120904002	1
Caelo	Triancinolona acetonido	1210-n09	1
Caelo	Triancinolona acetonido	1211013-01	1
Caelo	Triancinolona acetonido	12173701	5
Caelo	Triancinolona acetonido	12173703	1
Caelo	Triancinolona acetonido	12173704	1
Caelo	Triancinolona acetonido	12173705	2
Caelo	Triancinolona acetonido	12173707	5
Caelo	Triancinolona acetonido	12173710	5
Caelo	Triancinolona acetonido	12301501	4
Caelo	Triancinolona acetonido	12301502	1
Caelo	Triancinolona acetonido	12301503	1
Caelo	Triancinolona acetonido	12301504	1
Caelo	Triancinolona acetonido	12301505	1
Caelo	Triancinolona acetonido	12301506	1
Caelo	Triancinolona acetonido	12301507	8
Caelo	Triancinolona acetonido	12301508	4
Caelo	Triancinolona acetonido	12301509	4
Caelo	Triancinolona acetonido	12301510	4
Caelo	Triancinolona acetonido	12301515	12
Caelo	Triancinolona acetonido	12301518	4
Caelo	Triancinolona acetonido	1230517/16094502	1
Caelo	Triancinolona acetonido	1257952	1
Caelo	Triancinolona acetonido	12E15-N03	1
Caelo	Triancinolona acetonido	1303001-02	1
Caelo	Triancinolona acetonido	1312407	1
Caelo	Triancinolona acetonido	13124801	6
Caelo	Triancinolona acetonido	13124803	2
Caelo	Triancinolona acetonido	13124804	14
Caelo	Triancinolona acetonido	13124805	7
Caelo	Triancinolona acetonido	13124806	2
Caelo	Triancinolona acetonido	13124807	12
Caelo	Triancinolona acetonido	13124808	13
Caelo	Triancinolona acetonido	13124809	1
Caelo	Triancinolona acetonido	13124810	2
Caelo	Triancinolona acetonido	13124811	4
Caelo	Triancinolona acetonido	13256603	1
Caelo	Triancinolona acetonido	13256604	6
Caelo	Triancinolona acetonido	13256607	5
Caelo	Triancinolona acetonido	13256608	2
Caelo	Triancinolona acetonido	13379901	1
Caelo	Triancinolona acetonido	13379903	2
Caelo	Triancinolona acetonido	13379904	6
Caelo	Triancinolona acetonido	13379905	19
Caelo	Triancinolona acetonido	13379906	6
Caelo	Triancinolona acetonido	13379911	1
Caelo	Triancinolona acetonido	13379912	10
Caelo	Triancinolona acetonido	13379913	4
Caelo	Triancinolona acetonido	13379914	6
Caelo	Triancinolona acetonido	13379919	1
Caelo	Triancinolona acetonido	13379921	1
Caelo	Triancinolona acetonido	13379922	1
Caelo	Triancinolona acetonido	1355101	1
Caelo	Triancinolona acetonido	13C13-N20	2
Caelo	Triancinolona acetonido	13e15-n03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triancinolona acetonido	13E15-N03	2
Caelo	Triancinolona acetonido	13I26-N11	1
Caelo	Triancinolona acetonido	13K14-B04-289032	1
Caelo	Triancinolona acetonido	13K14-B04-289033	2
Caelo	Triancinolona acetonido	13K15-B31-289027	2
Caelo	Triancinolona acetonido	13K15-B31-289029	1
Caelo	Triancinolona acetonido	13K15-B31-289031	1
Caelo	Triancinolona acetonido	14188302	5
Caelo	Triancinolona acetonido	14188303	4
Caelo	Triancinolona acetonido	14188304	4
Caelo	Triancinolona acetonido	14233904	1
Caelo	Triancinolona acetonido	14255104	1
Caelo	Triancinolona acetonido	14355101	12
Caelo	Triancinolona acetonido	14355102	18
Caelo	Triancinolona acetonido	14355103	12
Caelo	Triancinolona acetonido	14355104	2
Caelo	Triancinolona acetonido	14355701	1
Caelo	Triancinolona acetonido	14355702	11
Caelo	Triancinolona acetonido	14355703	3
Caelo	Triancinolona acetonido	14355704	3
Caelo	Triancinolona acetonido	14355706	1
Caelo	Triancinolona acetonido	14355708	11
Caelo	Triancinolona acetonido	14355709	2
Caelo	Triancinolona acetonido	14355711	9
Caelo	Triancinolona acetonido	14355712	7
Caelo	Triancinolona acetonido	14G23_B07_2976618	1
Caelo	Triancinolona acetonido	14G23-B07-297619	1
Caelo	Triancinolona acetonido	1504007-01	1
Caelo	Triancinolona acetonido	1504007-02	1
Caelo	Triancinolona acetonido	1504007-2	1
Caelo	Triancinolona acetonido	1508008-01	2
Caelo	Triancinolona acetonido	1508008-02	1
Caelo	Triancinolona acetonido	1514Q2516	1
Caelo	Triancinolona acetonido	15233901	15
Caelo	Triancinolona acetonido	15233902	29
Caelo	Triancinolona acetonido	15233903	27
Caelo	Triancinolona acetonido	15233903-20160615Ma9	1
Caelo	Triancinolona acetonido	15233904	14
Caelo	Triancinolona acetonido	15233905	7
Caelo	Triancinolona acetonido	15233906	17
Caelo	Triancinolona acetonido	15233908	3
Caelo	Triancinolona acetonido	15233909	1
Caelo	Triancinolona acetonido	1530102	1
Caelo	Triancinolona acetonido	15308613	1
Caelo	Triancinolona acetonido	15430102	1
Caelo	Triancinolona acetonido	15430102I-300916/1	1
Caelo	Triancinolona acetonido	15430103	7
Caelo	Triancinolona acetonido	15430105	7
Caelo	Triancinolona acetonido	15430106	5
Caelo	Triancinolona acetonido	15430107	15
Caelo	Triancinolona acetonido	15430108	13
Caelo	Triancinolona acetonido	15C19-B06-308571	1
Caelo	Triancinolona acetonido	15C19-B06-308573	1
Caelo	Triancinolona acetonido	15G31-B07-313597	1
Caelo	Triancinolona acetonido	15G31-B07-314045	1
Caelo	Triancinolona acetonido	15L21-B03-316123	1
Caelo	Triancinolona acetonido	15L21-B03-318663	1
Caelo	Triancinolona acetonido	160102101	1
Caelo	Triancinolona acetonido	1601021-01	1
Caelo	Triancinolona acetonido	160501001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triancinolona acetonido	1605010-01	1
Caelo	Triancinolona acetonido	16079502	1
Caelo	Triancinolona acetonido	160800501	1
Caelo	Triancinolona acetonido	1608005-01	8
Caelo	Triancinolona acetonido	16092504	24
Caelo	Triancinolona acetonido	16094501	10
Caelo	Triancinolona acetonido	16094502	2
Caelo	Triancinolona acetonido	16094504	6
Caelo	Triancinolona acetonido	16094505	2
Caelo	Triancinolona acetonido	16094506	8
Caelo	Triancinolona acetonido	16094507	5
Caelo	Triancinolona acetonido	16094511	17
Caelo	Triancinolona acetonido	16094512	5
Caelo	Triancinolona acetonido	16094513	1
Caelo	Triancinolona acetonido	16094514	28
Caelo	Triancinolona acetonido	1612014	1
Caelo	Triancinolona acetonido	1612014-01	8
Caelo	Triancinolona acetonido	16B04-B07-318957	1
Caelo	Triancinolona acetonido	16D14-B11	1
Caelo	Triancinolona acetonido	16D14-B11-321318	1
Caelo	Triancinolona acetonido	16D14-B11-325482	2
Caelo	Triancinolona acetonido	16D14-B11-328167	1
Caelo	Triancinolona acetonido	16D16-B11-325482	1
Caelo	Triancinolona acetonido	16K07-B06-329447	1
Caelo	Triancinolona acetonido	16K07-B06-332102	1
Caelo	Triancinolona acetonido	16K07-B06-333438	3
Caelo	Triancinolona acetonido	17030347-01	1
Caelo	Triancinolona acetonido	1703037	1
Caelo	Triancinolona acetonido	170303701	2
Caelo	Triancinolona acetonido	1703037-01	2
Caelo	Triancinolona acetonido	170324T1612014-01	1
Caelo	Triancinolona acetonido	170547902	1
Caelo	Triancinolona acetonido	17057901	10
Caelo	Triancinolona acetonido	17057902	19
Caelo	Triancinolona acetonido	17057903	2
Caelo	Triancinolona acetonido	17057905	18
Caelo	Triancinolona acetonido	17057906	16
Caelo	Triancinolona acetonido	17057907	9
Caelo	Triancinolona acetonido	17057908	19
Caelo	Triancinolona acetonido	17057909	2
Caelo	Triancinolona acetonido	17057910	1
Caelo	Triancinolona acetonido	1705797	1
Caelo	Triancinolona acetonido	1706013-01	5
Caelo	Triancinolona acetonido	17060131	1
Caelo	Triancinolona acetonido	1706601-01	1
Caelo	Triancinolona acetonido	1710002-01	1
Caelo	Triancinolona acetonido	17100201	1
Caelo	Triancinolona acetonido	1710610	1
Caelo	Triancinolona acetonido	17120603	25
Caelo	Triancinolona acetonido	17120604	7
Caelo	Triancinolona acetonido	17120605	11
Caelo	Triancinolona acetonido	17120606	21
Caelo	Triancinolona acetonido	17120606/1211117	1
Caelo	Triancinolona acetonido	17120607	9
Caelo	Triancinolona acetonido	17120608	17
Caelo	Triancinolona acetonido	17120609	1
Caelo	Triancinolona acetonido	17120610	18
Caelo	Triancinolona acetonido	17120611	35
Caelo	Triancinolona acetonido	17120618	6
Caelo	Triancinolona acetonido	17120619	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triancinolona acetonido	17120620	11
Caelo	Triancinolona acetonido	17128606	1
Caelo	Triancinolona acetonido	1720606	1
Caelo	Triancinolona acetonido	1720608	1
Caelo	Triancinolona acetonido	1735302	1
Caelo	Triancinolona acetonido	17356306	1
Caelo	Triancinolona acetonido	1735802	1
Caelo	Triancinolona acetonido	1735805	1
Caelo	Triancinolona acetonido	17358302	47
Caelo	Triancinolona acetonido	17358302-T20181115Ma	1
Caelo	Triancinolona acetonido	17358303	8
Caelo	Triancinolona acetonido	17358304	14
Caelo	Triancinolona acetonido	17358305	40
Caelo	Triancinolona acetonido	17358309	2
Caelo	Triancinolona acetonido	1738305	1
Caelo	Triancinolona acetonido	17C09-B01-340173	1
Caelo	Triancinolona acetonido	17c09-b01-340174	1
Caelo	Triancinolona acetonido	17C09-B01-340174	2
Caelo	Triancinolona acetonido	17H03-B12-343457	1
Caelo	Triancinolona acetonido	17H03-B12-343459	1
Caelo	Triancinolona acetonido	17H03-B12-345552	1
Caelo	Triancinolona acetonido	17H03B12346697	1
Caelo	Triancinolona acetonido	180102001	2
Caelo	Triancinolona acetonido	1801020-01	6
Caelo	Triancinolona acetonido	18010202-01	1
Caelo	Triancinolona acetonido	1805001-01	7
Caelo	Triancinolona acetonido	180500102	1
Caelo	Triancinolona acetonido	1805001-02	2
Caelo	Triancinolona acetonido	1810015-01	2
Caelo	Triancinolona acetonido	18100203	11
Caelo	Triancinolona acetonido	18100204	18
Caelo	Triancinolona acetonido	18100205	14
Caelo	Triancinolona acetonido	18100206	9
Caelo	Triancinolona acetonido	18100207	3
Caelo	Triancinolona acetonido	18100208	10
Caelo	Triancinolona acetonido	18100209	12
Caelo	Triancinolona acetonido	18100210	30
Caelo	Triancinolona acetonido	18100213	28
Caelo	Triancinolona acetonido	18100215	1
Caelo	Triancinolona acetonido	18100217	5
Caelo	Triancinolona acetonido	18100218	4
Caelo	Triancinolona acetonido	18100220	21
Caelo	Triancinolona acetonido	18100221	30
Caelo	Triancinolona acetonido	18100222	23
Caelo	Triancinolona acetonido	18100225	3
Caelo	Triancinolona acetonido	18100226	22
Caelo	Triancinolona acetonido	1810207	1
Caelo	Triancinolona acetonido	1810299	1
Caelo	Triancinolona acetonido	1811211	1
Caelo	Triancinolona acetonido	18C15-B05-347275	1
Caelo	Triancinolona acetonido	18C15-B05-349087	1
Caelo	Triancinolona acetonido	18F14-B01-351889	1
Caelo	Triancinolona acetonido	18F14-B01-352343	1
Caelo	Triancinolona acetonido	18F14B01355979	1
Caelo	Triancinolona acetonido	18F14-B01-355979	1
Caelo	Triancinolona acetonido	18F14-B01-356853	1
Caelo	Triancinolona acetonido	1903015_01	1
Caelo	Triancinolona acetonido	1903015-01	1
Caelo	Triancinolona acetonido	1907044-01	2
Caelo	Triancinolona acetonido	1912005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triancinolona acetonido	191202003	2
Caelo	Triancinolona acetonido	191202005	28
Caelo	Triancinolona acetonido	191202006	20
Caelo	Triancinolona acetonido	191202007	8
Caelo	Triancinolona acetonido	19120205	1
Caelo	Triancinolona acetonido	19120205P-191111-2	1
Caelo	Triancinolona acetonido	19120206	12
Caelo	Triancinolona acetonido	19120207	35
Caelo	Triancinolona acetonido	19120208	27
Caelo	Triancinolona acetonido	19120209	38
Caelo	Triancinolona acetonido	19120210	22
Caelo	Triancinolona acetonido	1912021007	1
Caelo	Triancinolona acetonido	19120211	23
Caelo	Triancinolona acetonido	1912208	1
Caelo	Triancinolona acetonido	19J11-F02-367962	1
Caelo	Triancinolona acetonido	200000461003	1
Caelo	Triancinolona acetonido	200002630005	1
Caelo	Triancinolona acetonido	200002630006	2
Caelo	Triancinolona acetonido	20000461003	19
Caelo	Triancinolona acetonido	20000461004	21
Caelo	Triancinolona acetonido	20000461005	20
Caelo	Triancinolona acetonido	20000461006	9
Caelo	Triancinolona acetonido	20000461007	18
Caelo	Triancinolona acetonido	20000461010	1
Caelo	Triancinolona acetonido	20002360006	1
Caelo	Triancinolona acetonido	20002630001	4
Caelo	Triancinolona acetonido	20002630002	7
Caelo	Triancinolona acetonido	20002630003	1
Caelo	Triancinolona acetonido	20002630004	1
Caelo	Triancinolona acetonido	20002630005	36
Caelo	Triancinolona acetonido	20002630006	12
Caelo	Triancinolona acetonido	2000263005	1
Caelo	Triancinolona acetonido	20004422002	2
Caelo	Triancinolona acetonido	2000461006	1
Caelo	Triancinolona acetonido	2000461007	1
Caelo	Triancinolona acetonido	2000464005	1
Caelo	Triancinolona acetonido	2001017-01	1
Caelo	Triancinolona acetonido	2006002-01	4
Caelo	Triancinolona acetonido	2006032-01	1
Caelo	Triancinolona acetonido	201200601	1
Caelo	Triancinolona acetonido	2012006-01	4
Caelo	Triancinolona acetonido	20B28-F04-371546	3
Caelo	Triancinolona acetonido	20L18-F01-376650	1
Caelo	Triancinolona acetonido	210000116002	1
Caelo	Triancinolona acetonido	210000116014	1
Caelo	Triancinolona acetonido	21000116001	47
Caelo	Triancinolona acetonido	21000116002	15
Caelo	Triancinolona acetonido	21000116003	2
Caelo	Triancinolona acetonido	21000116004	1
Caelo	Triancinolona acetonido	21000116005	19
Caelo	Triancinolona acetonido	21000116006	4
Caelo	Triancinolona acetonido	21000116008	5
Caelo	Triancinolona acetonido	21000116010	4
Caelo	Triancinolona acetonido	21000116011	14
Caelo	Triancinolona acetonido	21000116014	24
Caelo	Triancinolona acetonido	21000116016	1
Caelo	Triancinolona acetonido	21000116018	1
Caelo	Triancinolona acetonido	21000116019	15
Caelo	Triancinolona acetonido	21000116021	1
Caelo	Triancinolona acetonido	21000116022	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triancinolona acetonido	21000118001	1
Caelo	Triancinolona acetonido	21000166001	1
Caelo	Triancinolona acetonido	21000428001	1
Caelo	Triancinolona acetonido	2100116014	1
Caelo	Triancinolona acetonido	2100303011	1
Caelo	Triancinolona acetonido	21003090310	1
Caelo	Triancinolona acetonido	21003093001	26
Caelo	Triancinolona acetonido	21003093003	11
Caelo	Triancinolona acetonido	21003093008	7
Caelo	Triancinolona acetonido	21003093009	1
Caelo	Triancinolona acetonido	21003093010	7
Caelo	Triancinolona acetonido	21003093011	15
Caelo	Triancinolona acetonido	2109004-02	1
Caelo	Triancinolona acetonido	22000902001	16
Caelo	Triancinolona acetonido	22000902002	12
Caelo	Triancinolona acetonido	22000902004	5
Caelo	Triancinolona acetonido	22000902005	9
Caelo	Triancinolona acetonido	22000902007	1
Caelo	Triancinolona acetonido	22000902008	2
Caelo	Triancinolona acetonido	22000902010	3
Caelo	Triancinolona acetonido	2208004-01	1
Caelo	Triancinolona acetonido	2211171	1
Caelo	Triancinolona acetonido	2449210001161	1
Caelo	Triancinolona acetonido	2513M02516	1
Caelo	Triancinolona acetonido	29091806	1
Caelo	Triancinolona acetonido	3041206	1
Caelo	Triancinolona acetonido	310320161	1
Caelo	Triancinolona acetonido	3110120	2
Caelo	Triancinolona acetonido	31117-1/16094502	1
Caelo	Triancinolona acetonido	3282	1
Caelo	Triancinolona acetonido	3340	1
Caelo	Triancinolona acetonido	42(18100213)	1
Caelo	Triancinolona acetonido	4613E2516	1
Caelo	Triancinolona acetonido	5430105	1
Caelo	Triancinolona acetonido	6051401	1
Caelo	Triancinolona acetonido	618E-02516	1
Caelo	Triancinolona acetonido	8681	1
Caelo	Triancinolona acetonido	9081305	1
Caelo	Triancinolona acetonido	912020061	1
Caelo	Triancinolona acetonido	93/AD1	1
Caelo	Triancinolona acetonido	9364429	2
Caelo	Triancinolona acetonido	95/AKD34	1
Caelo	Triancinolona acetonido	I270715-1	1
Caelo	Triancinolona acetonido	NA0088M	1
Caelo	Triancinolona acetonido	NS0571M	1
Caelo	Triancinolona acetonido	NZ0071M	1
Caesar & Loretz / Noweda	Triancinolona acetonido	191202006	1
Caesar & Loretz /Phönix	Triancinolona acetonido	21000116014	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120207	2
Caesar & Loretz GmbH...	Triancinolona acetonido	19120210	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120208	1
Caesar & Loretz GmbH...	Triancinolona acetonido	18100221	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461005	2
Caesar & Loretz GmbH...	Triancinolona acetonido	13379905	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461003	1
Caesar & Loretz GmbH...	Triancinolona acetonido	17358309	2
Caesar & Loretz GmbH...	Triancinolona acetonido	20002630006	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116011	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120208	1
Caesar & Loretz GmbH...	Triancinolona acetonido	22000902009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Triancinolona acetonido	19120208	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461005	1
Caesar & Loretz GmbH/AEP	Triancinolona acetonido	21003093001	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116014	1
Caesar & Loretz GmbH...	Triancinolona acetonido	191202005	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116002	1
Caesar & Loretz GmbH/Gehe	Triancinolona acetonido	18100210	1
Caesar & Loretz GmbH/Gehe	Triancinolona acetonido	18100220	1
Caesar & Loretz GmbH/GEHE	Triancinolona acetonido	21000116002	1
Caesar & Loretz GmbH/Gehe	Triancinolona acetonido	22000902016	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120207	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116002	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21003093003	2
Caesar & Loretz GmbH/Gö	Triancinolona acetonido	21003093011	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120210	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120211	5
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461007	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116005	2
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116019	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21003093010	1
Caesar & Loretz GmbH...	Triancinolona acetonido	22000902005	1
Caesar & Loretz GmbH...	Triancinolona acetonido	18100222	1
Caesar & Loretz GmbH...	Triancinolona acetonido	191202006	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461006	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20002630006	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20002630005	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116001	2
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116022	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21003093003	1
Caesar & Loretz GmbH...	Triancinolona acetonido	22000902001	1
Caesar & Loretz GmbH...	Triancinolona acetonido	18100209	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461005	1
Caesar & Loretz GmbH...	Triancinolona acetonido	18100210	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120211	2
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461006	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461007	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116008	1
Caesar & Loretz GmbH...	Triancinolona acetonido	18100210	1
Caesar & Loretz GmbH...	Triancinolona acetonido	19120207	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21003093011	1
Caesar & Loretz GmbH/Ph	Triancinolona acetonido	19120208	1
Caesar & Loretz GmbH/phö	Triancinolona acetonido	20000461003	2
Caesar & Loretz GmbH...	Triancinolona acetonido	20002630006	1
Caesar & Loretz GmbH...	Triancinolona acetonido	18100213	1
Caesar & Loretz GmbH...	Triancinolona acetonido	20000461007	2
Caesar & Loretz GmbH...	Triancinolona acetonido	20002630005	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116002	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116014	2
Caesar & Loretz GmbH...	Triancinolona acetonido	19120207	1
Caesar & Loretz GmbH...	Triancinolona acetonido	21000116001	2
Caesar & Loretz GmbH...	Triancinolona acetonido	21003093001	2
Caesar & Loretz GmbH	Triancinolona acetonido	17057906	1
Caesar & Loretz GmbH	Triancinolona acetonido	17057907	1
Caesar & Loretz GmbH	Triancinolona acetonido	17120610	1
Caesar & Loretz GmbH	Triancinolona acetonido	17358302	1
Caesar & Loretz GmbH	Triancinolona acetonido	17358305	2
Caesar & Loretz GmbH	Triancinolona acetonido	17358309	1
Caesar & Loretz GmbH	Triancinolona acetonido	175358305	1
Caesar & Loretz GmbH	Triancinolona acetonido	18100203	3
Caesar & Loretz GmbH	Triancinolona acetonido	18100206	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Triancinolona acetonido	18100209	1
Caesar & Loretz GmbH	Triancinolona acetonido	18100210	3
Caesar & Loretz GmbH	Triancinolona acetonido	18100213	4
Caesar & Loretz GmbH	Triancinolona acetonido	18100218	1
Caesar & Loretz GmbH	Triancinolona acetonido	18100220	2
Caesar & Loretz GmbH	Triancinolona acetonido	18100221	4
Caesar & Loretz GmbH	Triancinolona acetonido	18100222	5
Caesar & Loretz GmbH	Triancinolona acetonido	18100226	2
Caesar & Loretz GmbH	Triancinolona acetonido	1907044-01	1
Caesar & Loretz GmbH	Triancinolona acetonido	191202005	2
Caesar & Loretz GmbH	Triancinolona acetonido	191202006	3
Caesar & Loretz GmbH	Triancinolona acetonido	19120206	4
Caesar & Loretz GmbH	Triancinolona acetonido	19120207	3
Caesar & Loretz GmbH	Triancinolona acetonido	19120208	8
Caesar & Loretz GmbH	Triancinolona acetonido	19120209	8
Caesar & Loretz GmbH	Triancinolona acetonido	19120210	3
Caesar & Loretz GmbH	Triancinolona acetonido	19120211	3
Caesar & Loretz GmbH	Triancinolona acetonido	20000461003	6
Caesar & Loretz GmbH	Triancinolona acetonido	20000461004	4
Caesar & Loretz GmbH	Triancinolona acetonido	20000461005	8
Caesar & Loretz GmbH	Triancinolona acetonido	20000461006	7
Caesar & Loretz GmbH	Triancinolona acetonido	20000461007	4
Caesar & Loretz GmbH	Triancinolona acetonido	20002630001	5
Caesar & Loretz GmbH	Triancinolona acetonido	20002630002	1
Caesar & Loretz GmbH	Triancinolona acetonido	20002630005	6
Caesar & Loretz GmbH	Triancinolona acetonido	20002630006	9
Caesar & Loretz GmbH	Triancinolona acetonido	20004422002	1
Caesar & Loretz GmbH	Triancinolona acetonido	2002047-01	1
Caesar & Loretz GmbH	Triancinolona acetonido	2012006-01	2
Caesar & Loretz GmbH	Triancinolona acetonido	21000116001	22
Caesar & Loretz GmbH	Triancinolona acetonido	21000116002	14
Caesar & Loretz GmbH	Triancinolona acetonido	21000116005	4
Caesar & Loretz GmbH	Triancinolona acetonido	21000116006	2
Caesar & Loretz GmbH	Triancinolona acetonido	21000116008	6
Caesar & Loretz GmbH	Triancinolona acetonido	21000116011	4
Caesar & Loretz GmbH	Triancinolona acetonido	21000116012	1
Caesar & Loretz GmbH	Triancinolona acetonido	21000116013	2
Caesar & Loretz GmbH	Triancinolona acetonido	21000116014	14
Caesar & Loretz GmbH	Triancinolona acetonido	21000116018	4
Caesar & Loretz GmbH	Triancinolona acetonido	21000116019	6
Caesar & Loretz GmbH	Triancinolona acetonido	21000116022	1
Caesar & Loretz GmbH	Triancinolona acetonido	21003093001	9
Caesar & Loretz GmbH	Triancinolona acetonido	21003093003	4
Caesar & Loretz GmbH	Triancinolona acetonido	21003093008	9
Caesar & Loretz GmbH	Triancinolona acetonido	21003093009	1
Caesar & Loretz GmbH	Triancinolona acetonido	21003093010	2
Caesar & Loretz GmbH	Triancinolona acetonido	21003093011	3
Caesar & Loretz GmbH	Triancinolona acetonido	21003093012	1
Caesar & Loretz GmbH	Triancinolona acetonido	22000902001	6
Caesar & Loretz GmbH	Triancinolona acetonido	22000902004	3
Caesar & Loretz GmbH	Triancinolona acetonido	22000902005	2
Caesar & Loretz GmbH	Triancinolona acetonido	22000902009	5
Caesar & Loretz GmbH	Triancinolona acetonido	3695669	1
Caesar & Loretz	Triancinolona acetonido	17057906	1
Caesar & Loretz	Triancinolona acetonido	18100204	1
Caesar&loretz,Phoenix	Triancinolona acetonido	11267705	1
Caesar&loretz,Phoenix	Triancinolona acetonido	12173703	1
Caesar&loretz,Phoenix	Triancinolona acetonido	12301502	1
Caleo/ Noweda	Triancinolona acetonido	16092504	1
Caleo/ Noweda	Triancinolona acetonido	18100213	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caleo/Phönix	Triancinolona acetonido	21003093010	2
Calo, Hilden/ Phönix	Triancinolona acetonido	19120208	1
Calo/Sanacorp	Triancinolona acetonido	16092504	1
Cealo / Phönix / 22...	Triancinolona acetonido	18100225	1
Cealo/ AHD	Triancinolona acetonido	18100221	1
Cealo/Jenne	Triancinolona acetonido	220826(21003093001)	1
Cealo/Phönix	Triancinolona acetonido	17057901	1
Cealo	Triancinolona acetonido	1907044-01	1
Cealo	Triancinolona acetonido	20000461006	1
Cealo	Triancinolona acetonido	21000116005	1
cesar&lorentz/Phönix	Triancinolona acetonido	13124801	1
Christal Pharma/Ober...	Triancinolona acetonido	U0544/113530	1
Crystal Pharma /Ober...	Triancinolona acetonido	B0544/114010	2
Crystal pharma/ Ober...	Triancinolona acetonido	U0544/113530	1
Dr. Wolff	Triancinolona acetonido	1612014-01	1
Ebert & Jacobi	Triancinolona acetonido	16K07-B06-329445	1
Eigen/Defektur	Triancinolona acetonido	U0544/113530	1
E-plus	Triancinolona acetonido	17120610	2
EuRho / 11	Triancinolona acetonido	2006032-01	1
EuRho / Alliance	Triancinolona acetonido	2012006-01	1
Eurho / Alliance	Triancinolona acetonido	2109004-01	1
EuRho / Phoenix	Triancinolona acetonido	1612014-01	1
EuRho- Phoenix	Triancinolona acetonido	1710002-01	1
EuRho- Phoenix	Triancinolona acetonido	1810015-01	2
EuRho/ AHD	Triancinolona acetonido	1710002-01	1
EuRho/ Phönix	Triancinolona acetonido	1907044-01	1
EuRho/ Sanacorp	Triancinolona acetonido	1703037-01	1
EuRho/ Sanacorp	Triancinolona acetonido	2109004-01	1
EuRho/Noweda	Triancinolona acetonido	1601021-01	1
EuRho/Noweda	Triancinolona acetonido	1706013-01	1
EuRho/Noweda	Triancinolona acetonido	1710002-01	1
Eurho/Noweda	Triancinolona acetonido	2012006-01	1
EuRho/Phoenix	Triancinolona acetonido	1403009-02	1
EuRho/Phoenix	Triancinolona acetonido	2109004-03	1
EuRho/Phönix	Triancinolona acetonido	1211013-01	1
EuRho/Phönix	Triancinolona acetonido	1307043-02	1
EuRho/Phönix	Triancinolona acetonido	1407044-01	1
Eurho/Phönix	Triancinolona acetonido	2002047-01	1
Eurho/Phönix	Triancinolona acetonido	201200601	1
EuRho/Px	Triancinolona acetonido	219004-02	1
Eurho/Sanacorp	Triancinolona acetonido	1710002-01	1
EuRho/Sanacorp	Triancinolona acetonido	2006002-01	1
EuRho	Triancinolona acetonido	110015-01	1
EuRho	Triancinolona acetonido	1403009-02	1
EuRho	Triancinolona acetonido	1407044-02	1
EuRho	Triancinolona acetonido	150800-08-02	1
EuRho	Triancinolona acetonido	1508008-02	2
EuRho	Triancinolona acetonido	1703037-01	2
EuRho	Triancinolona acetonido	1706013-01	2
EuRho	Triancinolona acetonido	17100002-01	1
EuRho	Triancinolona acetonido	171000201	1
EuRho	Triancinolona acetonido	17100201	1
EuRho	Triancinolona acetonido	180500101	1
Eurho	Triancinolona acetonido	1805001-02	1
EuRho	Triancinolona acetonido	1810015-01	1
EuRho	Triancinolona acetonido	1905015-01	1
EuRho	Triancinolona acetonido	1907044-01	2
euRho	Triancinolona acetonido	2006032-01	1
EuRho	Triancinolona acetonido	2006032-01	2
EuRho	Triancinolona acetonido	2012006-01	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Triancinolona acetonido	2012006-02	1
EuRho	Triancinolona acetonido	NW2518M	1
Euro / Noweda	Triancinolona acetonido	1612014-01	1
Euro OCT / Krieger	Triancinolona acetonido	2002047-01	1
Euro OCT / Krieger	Triancinolona acetonido	2006032-01	1
Euro OTC	Triancinolona acetonido		5
Euro OTC	Triancinolona acetonido	1/10002-01	1
Euro OTC	Triancinolona acetonido	1013I-02516	1
Euro OTC	Triancinolona acetonido	1110005-01	2
Euro OTC	Triancinolona acetonido	111005-01	1
Euro OTC	Triancinolona acetonido	1112023-01	1
Euro OTC	Triancinolona acetonido	1112023-02	6
Euro OTC	Triancinolona acetonido	112014-01	1
Euro OTC	Triancinolona acetonido	11801020-01	1
Euro OTC	Triancinolona acetonido	1206008-01	5
Euro OTC	Triancinolona acetonido	1209040-01	4
Euro OTC	Triancinolona acetonido	1209040-02	2
Euro OTC	Triancinolona acetonido	1211013-01	4
Euro OTC	Triancinolona acetonido	1211013-02	9
Euro OTC	Triancinolona acetonido	121113-02	1
Euro OTC	Triancinolona acetonido	1234567	1
Euro OTC	Triancinolona acetonido	12G6008-01	1
Euro OTC	Triancinolona acetonido	13030001-01	1
Euro OTC	Triancinolona acetonido	1303001-01	5
Euro OTC	Triancinolona acetonido	1303001-02	8
Euro OTC	Triancinolona acetonido	130704301	1
Euro OTC	Triancinolona acetonido	1307043-01	16
Euro OTC	Triancinolona acetonido	130704302	1
Euro OTC	Triancinolona acetonido	1307043-02	14
Euro OTC	Triancinolona acetonido	1307043-03	1
Euro OTC	Triancinolona acetonido	14030009-01	2
Euro OTC	Triancinolona acetonido	14030009-02	1
Euro OTC	Triancinolona acetonido	1403009-01	7
Euro OTC	Triancinolona acetonido	1403009-02	13
Euro OTC	Triancinolona acetonido	1407044-01	9
Euro OTC	Triancinolona acetonido	1407044-02	15
Euro OTC	Triancinolona acetonido	140744-02	1
Euro OTC	Triancinolona acetonido	14120130	1
Euro OTC	Triancinolona acetonido	141201301	1
Euro OTC	Triancinolona acetonido	1412013-01	13
Euro OTC	Triancinolona acetonido	141201302	4
Euro OTC	Triancinolona acetonido	1412013-02	9
Euro OTC	Triancinolona acetonido	141213-02	1
Euro OTC	Triancinolona acetonido	14188304	1
Euro OTC	Triancinolona acetonido	150400701	2
Euro OTC	Triancinolona acetonido	1504007-01	10
Euro OTC	Triancinolona acetonido	1504007-02	17
Euro OTC	Triancinolona acetonido	15041007-02	1
Euro OTC	Triancinolona acetonido	15042014A	1
Euro OTC	Triancinolona acetonido	1508008	1
Euro OTC	Triancinolona acetonido	1508008-01	17
Euro OTC	Triancinolona acetonido	150800802	2
Euro OTC	Triancinolona acetonido	1508008-02	16
Euro OTC	Triancinolona acetonido	15081701	1
Euro OTC	Triancinolona acetonido	15111740	1
Euro OTC	Triancinolona acetonido	15121806	1
Euro OTC	Triancinolona acetonido	15233904	1
Euro OTC	Triancinolona acetonido	15233906	2
Euro OTC	Triancinolona acetonido	15404007-01	1
Euro OTC	Triancinolona acetonido	15430103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triancinolona acetonido	15121-b03-316123	1
Euro OTC	Triancinolona acetonido	15L21-B03-316123	2
Euro OTC	Triancinolona acetonido	1601021-01	32
Euro OTC	Triancinolona acetonido	1602005-01	1
Euro OTC	Triancinolona acetonido	160501001	3
Euro OTC	Triancinolona acetonido	1605010-01	42
Euro OTC	Triancinolona acetonido	160510-01	1
Euro OTC	Triancinolona acetonido	1608005	1
Euro OTC	Triancinolona acetonido	1608005-01	44
Euro OTC	Triancinolona acetonido	161006T	1
Euro OTC	Triancinolona acetonido	1612014-01	64
Euro OTC	Triancinolona acetonido	1612014-014	1
Euro OTC	Triancinolona acetonido	161214-01	1
Euro OTC	Triancinolona acetonido	16D14-B11	1
Euro OTC	Triancinolona acetonido	16D14-B11-322136	1
Euro OTC	Triancinolona acetonido	170060013-01	1
Euro OTC	Triancinolona acetonido	17030307-01	1
Euro OTC	Triancinolona acetonido	1703037	3
Euro OTC	Triancinolona acetonido	1703037_01	1
Euro OTC	Triancinolona acetonido	170303701	3
Euro OTC	Triancinolona acetonido	1703037-01	56
Euro OTC	Triancinolona acetonido	1706013	1
Euro OTC	Triancinolona acetonido	170601301	5
Euro OTC	Triancinolona acetonido	1706013-01	71
Euro OTC	Triancinolona acetonido	1706079-01	1
Euro OTC	Triancinolona acetonido	17061406	1
Euro OTC	Triancinolona acetonido	171000-01	1
Euro OTC	Triancinolona acetonido	17100002-01	1
Euro OTC	Triancinolona acetonido	1710002-01	69
Euro OTC	Triancinolona acetonido	1710002-1	1
Euro OTC	Triancinolona acetonido	171002-01	2
Euro OTC	Triancinolona acetonido	171212T/1703037-01	1
Euro OTC	Triancinolona acetonido	171302-01	1
Euro OTC	Triancinolona acetonido	171613-01	1
Euro OTC	Triancinolona acetonido	1801020	3
Euro OTC	Triancinolona acetonido	180102001	3
Euro OTC	Triancinolona acetonido	1801020-01	80
Euro OTC	Triancinolona acetonido	1801020-1	1
Euro OTC	Triancinolona acetonido	1805001	1
Euro OTC	Triancinolona acetonido	180500101	3
Euro OTC	Triancinolona acetonido	1805001-01	43
Euro OTC	Triancinolona acetonido	180500102	1
Euro OTC	Triancinolona acetonido	1805001-02	24
Euro OTC	Triancinolona acetonido	1810015001	1
Euro OTC	Triancinolona acetonido	181001501	5
Euro OTC	Triancinolona acetonido	1810015-01	92
Euro OTC	Triancinolona acetonido	181016181	1
Euro OTC	Triancinolona acetonido	181020-1	1
Euro OTC	Triancinolona acetonido	190301501	1
Euro OTC	Triancinolona acetonido	1903015-01	64
Euro OTC	Triancinolona acetonido	1903015-15	1
Euro OTC	Triancinolona acetonido	19030156-01	1
Euro OTC	Triancinolona acetonido	190601206	1
Euro OTC	Triancinolona acetonido	190704401	5
Euro OTC	Triancinolona acetonido	1907044-01	82
Euro OTC	Triancinolona acetonido	19070744-01	1
Euro OTC	Triancinolona acetonido	19074401	1
Euro OTC	Triancinolona acetonido	190744-01	1
Euro OTC	Triancinolona acetonido	1912014-01	1
Euro OTC	Triancinolona acetonido	19120209	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triancinolona acetonido	20006032-01	1
Euro OTC	Triancinolona acetonido	2001017	1
Euro OTC	Triancinolona acetonido	2001017-01	7
Euro OTC	Triancinolona acetonido	2002047	3
Euro OTC	Triancinolona acetonido	200204701	5
Euro OTC	Triancinolona acetonido	2002047-01	49
Euro OTC	Triancinolona acetonido	20024047-01	1
Euro OTC	Triancinolona acetonido	200600201	1
Euro OTC	Triancinolona acetonido	2006002-01	56
Euro OTC	Triancinolona acetonido	2006002-1	1
Euro OTC	Triancinolona acetonido	200603201	1
Euro OTC	Triancinolona acetonido	2006032-01	53
Euro OTC	Triancinolona acetonido	2006032-31	1
Euro OTC	Triancinolona acetonido	2012	1
Euro OTC	Triancinolona acetonido	2012003-01	1
Euro OTC	Triancinolona acetonido	2012006	2
Euro OTC	Triancinolona acetonido	2012006_01	1
Euro OTC	Triancinolona acetonido	201200601	8
Euro OTC	Triancinolona acetonido	2012006-01	61
Euro OTC	Triancinolona acetonido	2012006-02	37
Euro OTC	Triancinolona acetonido	2012006-04	1
Euro OTC	Triancinolona acetonido	2012006-1	1
Euro OTC	Triancinolona acetonido	20130912-5	1
Euro OTC	Triancinolona acetonido	2015006-01	1
Euro OTC	Triancinolona acetonido	20212006-01	1
Euro OTC	Triancinolona acetonido	2108004-03	1
Euro OTC	Triancinolona acetonido	21090004-01	1
Euro OTC	Triancinolona acetonido	2109001-03	1
Euro OTC	Triancinolona acetonido	2109004_01	1
Euro OTC	Triancinolona acetonido	21090040-02	1
Euro OTC	Triancinolona acetonido	2109004-01	48
Euro OTC	Triancinolona acetonido	2109004-02	23
Euro OTC	Triancinolona acetonido	2109004-03	14
Euro OTC	Triancinolona acetonido	220800401	1
Euro OTC	Triancinolona acetonido	2208004-01	11
Euro OTC	Triancinolona acetonido	2208004-02	1
Euro OTC	Triancinolona acetonido	23061808	1
Euro OTC	Triancinolona acetonido	26011804	1
Euro OTC	Triancinolona acetonido	26081405	1
Euro OTC	Triancinolona acetonido	2772	1
Euro OTC	Triancinolona acetonido	28041728	1
Euro OTC	Triancinolona acetonido	2898	1
Euro OTC	Triancinolona acetonido	29011503	1
Euro OTC	Triancinolona acetonido	29081501	1
Euro OTC	Triancinolona acetonido	3022015A	1
Euro OTC	Triancinolona acetonido	3051402	1
Euro OTC	Triancinolona acetonido	31101414	1
Euro OTC	Triancinolona acetonido	5051816	1
Euro OTC	Triancinolona acetonido	6702020004	1
Euro OTC	Triancinolona acetonido	6702020010	2
Euro OTC	Triancinolona acetonido	6702021007	3
Euro OTC	Triancinolona acetonido	700124	1
Euro OTC	Triancinolona acetonido	8031803	1
Euro OTC	Triancinolona acetonido	80616-5	1
Euro OTC	Triancinolona acetonido	8700	1
Euro OTC	Triancinolona acetonido	APB0544/112020T	1
Euro OTC	Triancinolona acetonido	B0544/111404	1
Euro OTC	Triancinolona acetonido	NV0635M	1
Euro OTC	Triancinolona acetonido	NW2518M	1
Euro OTC	Triancinolona acetonido	NX2518M	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triancinolona acetonido	NZ032211	1
Euro OTC	Triancinolona acetonido	PT49	1
Euro/ Anzag	Triancinolona acetonido	2012006-02	1
euro/ Anzag	Triancinolona acetonido	3315I02516	1
Euro/Gehe	Triancinolona acetonido	1612014-01	1
Euro/Gehe	Triancinolona acetonido	1703037-01	1
Euro/gehe	Triancinolona acetonido	2012006-01	1
Euro/Krieger	Triancinolona acetonido	1907044-01	1
Euro/Noweda	Triancinolona acetonido	161201401	1
Euro/Phönix	Triancinolona acetonido	1805401	1
Euro/Phönix	Triancinolona acetonido	1907044	1
Euro/Sanacorp	Triancinolona acetonido	2006002-01	1
Euro/Sanacorp	Triancinolona acetonido	2008032-01	1
euro	Triancinolona acetonido	1211013-02	1
Euro	Triancinolona acetonido	1303001-02	1
euroct/gehe	Triancinolona acetonido	1403009	1
euroct/gehe	Triancinolona acetonido	1403009-02	1
EuroOCT/Gehe	Triancinolona acetonido	1710002-01	2
Europharm/Otto	Triancinolona acetonido	1206008-01	1
Europharm/Otto	Triancinolona acetonido	1209040-02	1
Europharm/Sanacorp	Triancinolona acetonido	1211013-01	3
Europharm/Sanacorp	Triancinolona acetonido	B0544/111040	2
Fagron	Triancinolona acetonido		3
Fagron	Triancinolona acetonido	11B22-N05	1
Fagron	Triancinolona acetonido	11K11-N10	6
Fagron	Triancinolona acetonido	11N11-N10	1
Fagron	Triancinolona acetonido	12/10-N09	4
Fagron	Triancinolona acetonido	12/-N09	1
Fagron	Triancinolona acetonido	120600801	1
Fagron	Triancinolona acetonido	1210-N09	1
Fagron	Triancinolona acetonido	12301503	1
Fagron	Triancinolona acetonido	12B08N01	1
Fagron	Triancinolona acetonido	12B08-N01	8
Fagron	Triancinolona acetonido	12E15/N03	1
Fagron	Triancinolona acetonido	12E15-N03	21
Fagron	Triancinolona acetonido	12I10-N09	4
Fagron	Triancinolona acetonido	12l10-N09	3
Fagron	Triancinolona acetonido	13/26-N11	7
Fagron	Triancinolona acetonido	13021408	1
Fagron	Triancinolona acetonido	13121201	1
Fagron	Triancinolona acetonido	13126-N11	1
Fagron	Triancinolona acetonido	1326-N11	1
Fagron	Triancinolona acetonido	13C13-20	1
Fagron	Triancinolona acetonido	13c13-n20	1
Fagron	Triancinolona acetonido	13C13-N20	14
Fagron	Triancinolona acetonido	13C13-N200217/412	1
Fagron	Triancinolona acetonido	13e15-n03	1
Fagron	Triancinolona acetonido	13E15N03	3
Fagron	Triancinolona acetonido	13E15-N03	44
Fagron	Triancinolona acetonido	13E15-NO3	1
Fagron	Triancinolona acetonido	13i26-N11	1
Fagron	Triancinolona acetonido	13I26N11	1
Fagron	Triancinolona acetonido	13I26-N11	13
Fagron	Triancinolona acetonido	13I26-N26	1
Fagron	Triancinolona acetonido	13K14-b04	1
Fagron	Triancinolona acetonido	13K14-B04	4
Fagron	Triancinolona acetonido	13k14-B04-289032	1
Fagron	Triancinolona acetonido	13K14-B04-289032	6
Fagron	Triancinolona acetonido	13K14-B04-289033	10
Fagron	Triancinolona acetonido	13K15-B31	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triancinolona acetonido	13K15-B31-289025	1
Fagron	Triancinolona acetonido	13K15-B31-289027	6
Fagron	Triancinolona acetonido	13K15B31289029	1
Fagron	Triancinolona acetonido	13K15-B31-289029	3
Fagron	Triancinolona acetonido	13k15-b31-289030	1
Fagron	Triancinolona acetonido	13K15-B31-289031	6
Fagron	Triancinolona acetonido	1407044-01	1
Fagron	Triancinolona acetonido	1412013-01	1
Fagron	Triancinolona acetonido	14355104	1
Fagron	Triancinolona acetonido	14355709	1
Fagron	Triancinolona acetonido	14F30B01	1
Fagron	Triancinolona acetonido	14F30-B01	2
Fagron	Triancinolona acetonido	14F30-B01-296287	4
Fagron	Triancinolona acetonido	14F30-B021-296287	1
Fagron	Triancinolona acetonido	14G23-B07	1
Fagron	Triancinolona acetonido	14G23-B07-297618	5
Fagron	Triancinolona acetonido	14G23-B07-297619	2
Fagron	Triancinolona acetonido	14G23-B07-297620	7
Fagron	Triancinolona acetonido	14G23-B07-297620	1
Fagron	Triancinolona acetonido	14k14-B05-302887	1
Fagron	Triancinolona acetonido	14K14-B05-302887	2
Fagron	Triancinolona acetonido	14K24N-N01	1
Fagron	Triancinolona acetonido	1508008-02	1
Fagron	Triancinolona acetonido	1531-07-313596	1
Fagron	Triancinolona acetonido	15B02-B03	5
Fagron	Triancinolona acetonido	15B02-B03-303827	2
Fagron	Triancinolona acetonido	15B02-B03-303828	5
Fagron	Triancinolona acetonido	15B02-B03-303830	8
Fagron	Triancinolona acetonido	15BO2-B03-303828	1
Fagron	Triancinolona acetonido	15C19-B06	1
Fagron	Triancinolona acetonido	15C19-B06-308571	1
Fagron	Triancinolona acetonido	15C19-B06-308572	7
Fagron	Triancinolona acetonido	15C19-B06-308573	9
Fagron	Triancinolona acetonido	15C19-B06-309194	2
Fagron	Triancinolona acetonido	15G31B07	2
Fagron	Triancinolona acetonido	15G31-B07	2
Fagron	Triancinolona acetonido	15G31-B07-313596	6
Fagron	Triancinolona acetonido	15G31B07313597	1
Fagron	Triancinolona acetonido	15G31-B07-313597	6
Fagron	Triancinolona acetonido	15G31-B07-314045	6
Fagron	Triancinolona acetonido	15g31-b07-314046	1
Fagron	Triancinolona acetonido	15G31-B07-314046	4
Fagron	Triancinolona acetonido	15G31-B07-314047	3
Fagron	Triancinolona acetonido	15L21-B03	1
Fagron	Triancinolona acetonido	15L21-B03-316123	8
Fagron	Triancinolona acetonido	15L21-B03-318663	4
Fagron	Triancinolona acetonido	16011407	1
Fagron	Triancinolona acetonido	16014-B12-3231318	1
Fagron	Triancinolona acetonido	1608005-01	1
Fagron	Triancinolona acetonido	1612014-01	1
Fagron	Triancinolona acetonido	16B04	1
Fagron	Triancinolona acetonido	16B04-B07	4
Fagron	Triancinolona acetonido	16B04-B07318664	1
Fagron	Triancinolona acetonido	16B04-B07-318664	7
Fagron	Triancinolona acetonido	16B04-B07-318957	6
Fagron	Triancinolona acetonido	16B04-B07-319471	4
Fagron	Triancinolona acetonido	16B04-Bo7-318664	1
Fagron	Triancinolona acetonido	16-B07-318664	1
Fagron	Triancinolona acetonido	16D04-B11-325479	1
Fagron	Triancinolona acetonido	16D14_B11_328167	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triancinolona acetonido	16D14-B11	2
Fagron	Triancinolona acetonido	16D14-B11_322158	1
Fagron	Triancinolona acetonido	16D14-B11-321318	3
Fagron	Triancinolona acetonido	16D14-B11-322135	4
Fagron	Triancinolona acetonido	16D14-B11-322136	9
Fagron	Triancinolona acetonido	16D14-B11-322158	10
Fagron	Triancinolona acetonido	16D14B11325479	1
Fagron	Triancinolona acetonido	16D14-B11-325479	6
Fagron	Triancinolona acetonido	16D14-B11-325480	3
Fagron	Triancinolona acetonido	16D14-B11-325481	1
Fagron	Triancinolona acetonido	16D14-B11-325482	7
Fagron	Triancinolona acetonido	16D14-B11-328167	14
Fagron	Triancinolona acetonido	16K07-B06	3
Fagron	Triancinolona acetonido	16K07-B060921	1
Fagron	Triancinolona acetonido	16K07B06329445	1
Fagron	Triancinolona acetonido	16K07-B06-329445	5
Fagron	Triancinolona acetonido	16K07-B06-329446	1
Fagron	Triancinolona acetonido	16K07-B06-329447	1
Fagron	Triancinolona acetonido	16K07-B06-332101	7
Fagron	Triancinolona acetonido	16K07-B06-332102	4
Fagron	Triancinolona acetonido	16k07-b06332103	1
Fagron	Triancinolona acetonido	16K07B06332103	1
Fagron	Triancinolona acetonido	16K07-B06-332103	2
Fagron	Triancinolona acetonido	16K07-B06-333438	4
Fagron	Triancinolona acetonido	16l07-b06-332102	1
Fagron	Triancinolona acetonido	1703-B12-345553	1
Fagron	Triancinolona acetonido	17C09_B01_337464	1
Fagron	Triancinolona acetonido	17C09-B01	3
Fagron	Triancinolona acetonido	17C09-B01_337464	1
Fagron	Triancinolona acetonido	17C09-B01-334196	6
Fagron	Triancinolona acetonido	17C09-B01-334197	4
Fagron	Triancinolona acetonido	17C-09-B01-334197	1
Fagron	Triancinolona acetonido	17C09-B01-336881	2
Fagron	Triancinolona acetonido	17C09-B01-337464	3
Fagron	Triancinolona acetonido	17C09-B01-340173	10
Fagron	Triancinolona acetonido	17c09-b01-340174	1
Fagron	Triancinolona acetonido	17C09-B01-340174	10
Fagron	Triancinolona acetonido	17C-B01-336881	2
Fagron	Triancinolona acetonido	17F14-B01-352343	1
Fagron	Triancinolona acetonido	17H03-812-346697	1
Fagron	Triancinolona acetonido	17H03-B12	6
Fagron	Triancinolona acetonido	17H03-B12-343457	6
Fagron	Triancinolona acetonido	17H03-B12343458	1
Fagron	Triancinolona acetonido	17H03-B12-343458	6
Fagron	Triancinolona acetonido	17H03-B12-343459	3
Fagron	Triancinolona acetonido	17h03-b12-343672	1
Fagron	Triancinolona acetonido	17H03-B12-343672	6
Fagron	Triancinolona acetonido	17H03-B12-345552	10
Fagron	Triancinolona acetonido	17H03-B12-345553	2
Fagron	Triancinolona acetonido	17H03-B12-346697	2
Fagron	Triancinolona acetonido	17H03-B12-672	1
Fagron	Triancinolona acetonido	1810015-01	1
Fagron	Triancinolona acetonido	18100205	1
Fagron	Triancinolona acetonido	18100221	1
Fagron	Triancinolona acetonido	18C15-B05	6
Fagron	Triancinolona acetonido	18C15-B05_348063	1
Fagron	Triancinolona acetonido	18C15B05347275	2
Fagron	Triancinolona acetonido	18C15-B05-347275	6
Fagron	Triancinolona acetonido	18C15-B05-348063	6
Fagron	Triancinolona acetonido	18c15-b05-348064	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triancinolona acetonido	18C15-B05-348064	3
Fagron	Triancinolona acetonido	18c15-b05-349087	1
Fagron	Triancinolona acetonido	18C15-B05-349087	8
Fagron	Triancinolona acetonido	18c15-b05-350263	1
Fagron	Triancinolona acetonido	18C15-B05-350263	4
Fagron	Triancinolona acetonido	18C15-B05-348063	1
Fagron	Triancinolona acetonido	18F14	1
Fagron	Triancinolona acetonido	18F14_B01_352343	1
Fagron	Triancinolona acetonido	18F14_B01_352630	1
Fagron	Triancinolona acetonido	18F14-B01	3
Fagron	Triancinolona acetonido	18F14-B01_356853	1
Fagron	Triancinolona acetonido	18f14b01351889	1
Fagron	Triancinolona acetonido	18F14-B01-351889	7
Fagron	Triancinolona acetonido	18F14-B01-352343	10
Fagron	Triancinolona acetonido	18F14-B01-352630	5
Fagron	Triancinolona acetonido	18F14-B01-353255	9
Fagron	Triancinolona acetonido	18F14-B01-355724	4
Fagron	Triancinolona acetonido	18F14-B01-355979	5
Fagron	Triancinolona acetonido	18F14-B01-356853	13
Fagron	Triancinolona acetonido	18f14-b01-357073	1
Fagron	Triancinolona acetonido	18F14-B01-357073	6
Fagron	Triancinolona acetonido	18F14-B-351889	1
Fagron	Triancinolona acetonido	18F14-BO1-357073	1
Fagron	Triancinolona acetonido	18I216-B05-361518	1
Fagron	Triancinolona acetonido	18k16-B05	1
Fagron	Triancinolona acetonido	18K16-B05	5
Fagron	Triancinolona acetonido	18K-16-B05	1
Fagron	Triancinolona acetonido	18K16-B05_367959	1
Fagron	Triancinolona acetonido	18K16-B05-357775	4
Fagron	Triancinolona acetonido	18K16-B05-35969	1
Fagron	Triancinolona acetonido	18K16-B05-359867	7
Fagron	Triancinolona acetonido	18K16-B05-359868	6
Fagron	Triancinolona acetonido	18K16-B05-359869	4
Fagron	Triancinolona acetonido	18K16-B05-359871	8
Fagron	Triancinolona acetonido	18K16-B05-361518	6
Fagron	Triancinolona acetonido	18K16-B05-361521	8
Fagron	Triancinolona acetonido	18K16-B05-361522	2
Fagron	Triancinolona acetonido	18K-16-B05-361522	1
Fagron	Triancinolona acetonido	18k16b05361523	1
Fagron	Triancinolona acetonido	18k16-b05-361523	1
Fagron	Triancinolona acetonido	18K16-B05-361523	3
Fagron	Triancinolona acetonido	18K16-B05-367959	5
Fagron	Triancinolona acetonido	18K16-B06-357775	1
Fagron	Triancinolona acetonido	19J11-F02	2
Fagron	Triancinolona acetonido	19J11-F02-367958	1
Fagron	Triancinolona acetonido	19J11-F02367961	1
Fagron	Triancinolona acetonido	19J11-F02-367961	2
Fagron	Triancinolona acetonido	19J11-F02-367962	6
Fagron	Triancinolona acetonido	19J11-F02-368619	1
Fagron	Triancinolona acetonido	19J11-FO2-367958	1
Fagron	Triancinolona acetonido	19J-F02-367962	1
Fagron	Triancinolona acetonido	20031302	1
Fagron	Triancinolona acetonido	20828-F04-371546	1
Fagron	Triancinolona acetonido	20B28-F04	5
Fagron	Triancinolona acetonido	20B28-F04-0005	1
Fagron	Triancinolona acetonido	20B28-F04-3715406	1
Fagron	Triancinolona acetonido	20B28-F04-371541	7
Fagron	Triancinolona acetonido	20B28-F04-371542	1
Fagron	Triancinolona acetonido	20B28F04-371544	1
Fagron	Triancinolona acetonido	20B28-F04-371544	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triancinolona acetonido	20b28-f04-371546	1
Fagron	Triancinolona acetonido	20b28-F04-371546	1
Fagron	Triancinolona acetonido	20B28-F04-371546	15
Fagron	Triancinolona acetonido	20L18-F01	3
Fagron	Triancinolona acetonido	20L-18-F01	1
Fagron	Triancinolona acetonido	20l18-f01-376647	1
Fagron	Triancinolona acetonido	20L18-F01-376647	7
Fagron	Triancinolona acetonido	20L18-F01-376649	2
Fagron	Triancinolona acetonido	20L18-F01-376650	8
Fagron	Triancinolona acetonido	20L18-F01-376653	1
Fagron	Triancinolona acetonido	20L18F01-376658	1
Fagron	Triancinolona acetonido	20L18-F01-376658	3
Fagron	Triancinolona acetonido	20L18F01376658	1
Fagron	Triancinolona acetonido	21H04-B13-21363	1
Fagron	Triancinolona acetonido	21H04-B13-213632	1
Fagron	Triancinolona acetonido	21H04-B13-213633	3
Fagron	Triancinolona acetonido	21H25-F03-379863	5
Fagron	Triancinolona acetonido	21H25-F03-379867	7
Fagron	Triancinolona acetonido	21H25-F03-379871	3
Fagron	Triancinolona acetonido	21H25-F03-379874	15
Fagron	Triancinolona acetonido	21H25-F03-379875	13
Fagron	Triancinolona acetonido	21H25-FO3-379871	1
Fagron	Triancinolona acetonido	21J20-B03	2
Fagron	Triancinolona acetonido	21j20-b03-217884	1
Fagron	Triancinolona acetonido	21J20-B03-217884	7
Fagron	Triancinolona acetonido	21J20-Bo3-217884	1
Fagron	Triancinolona acetonido	21J20-BO3-217884	1
Fagron	Triancinolona acetonido	22A22-B01-218005	2
Fagron	Triancinolona acetonido	22A22-B01-218005/NB3123M	1
Fagron	Triancinolona acetonido	22D15-B01-220144	2
Fagron	Triancinolona acetonido	289027	1
Fagron	Triancinolona acetonido	3212U-02516(NP)	1
Fagron	Triancinolona acetonido	355724	1
Fagron	Triancinolona acetonido	411082-1-P	1
Fagron	Triancinolona acetonido	4111408	1
Fagron	Triancinolona acetonido	5061205	1
Fagron	Triancinolona acetonido	5061303	1
Fagron	Triancinolona acetonido	5121302	1
Fagron	Triancinolona acetonido	7041501	1
Fagron	Triancinolona acetonido	9041305	1
Fagron	Triancinolona acetonido	B05-3480603	1
Fagron	Triancinolona acetonido	B05-3598607	1
Fagron	Triancinolona acetonido	B053679509	1
Fagron	Triancinolona acetonido	C22H25CIN209	1
Fagron	Triancinolona acetonido	F01_3766500	1
Fagron	Triancinolona acetonido	F01-3766407	1
Fagron	Triancinolona acetonido	F01-3766507	1
Fagron	Triancinolona acetonido	F01-3766508	1
Fagron	Triancinolona acetonido	F01-376653	1
Fagron	Triancinolona acetonido	F02-3679508	1
Fagron	Triancinolona acetonido	F02-3679602	1
Fagron	Triancinolona acetonido	F03-3798603	1
Fagron	Triancinolona acetonido	F03-3798704	1
Fagron	Triancinolona acetonido	F04-3715401	1
Fagron	Triancinolona acetonido	F04-3715406	5
Fagron	Triancinolona acetonido	F08-3679508	1
Fagron	Triancinolona acetonido	FO1-3766507	1
Fagron	Triancinolona acetonido	NA0087M	3
Fagron	Triancinolona acetonido	NA3552M	6
Fagron	Triancinolona acetonido	NB0601M	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triancinolona acetonido	NBO601M	2
Fagron	Triancinolona acetonido	NS0571M	5
Fagron	Triancinolona acetonido	NS0996M	2
Fagron	Triancinolona acetonido	NS2236M	1
Fagron	Triancinolona acetonido	NSO571M	1
Fagron	Triancinolona acetonido	NT0487M	1
Fagron	Triancinolona acetonido	NT0770M	1
Fagron	Triancinolona acetonido	NT077oM	1
Fagron	Triancinolona acetonido	NT1094M	1
Fagron	Triancinolona acetonido	NT1430M	3
Fagron	Triancinolona acetonido	NU0930M	1
Fagron	Triancinolona acetonido	NVO262M	1
Fagron	Triancinolona acetonido	Nw0635M	1
Fagron	Triancinolona acetonido	NW2261M	2
Fagron	Triancinolona acetonido	NW2518M	1
Fagron	Triancinolona acetonido	NX0241M	1
Fagron	Triancinolona acetonido	NX1540M	2
Fagron	Triancinolona acetonido	ny0485m	1
Fagron	Triancinolona acetonido	NY0485M	5
Fagron	Triancinolona acetonido	NY1271M	6
Fagron	Triancinolona acetonido	NY2097M	2
Fargon / AHD	Triancinolona acetonido	18C15-B05-350263	1
Fargon/Alliance HC	Triancinolona acetonido	15B02-B03-303830	1
Fargon/Anzag	Triancinolona acetonido	13/26-N11	3
Fargon/Gehe	Triancinolona acetonido	16D14-B11	1
Fargon/Phoenix	Triancinolona acetonido	18K16-B05-359871	1
fargon	Triancinolona acetonido	13C13-N20	1
Fargon	Triancinolona acetonido	15C19-B06-308572	2
Fargon	Triancinolona acetonido	15C19-B06-308573	1
Fargon	Triancinolona acetonido	Nu2526M	1
Fargron	Triancinolona acetonido	13/26-N11	1
Farmabios / Gehe	Triancinolona acetonido	15233905	1
Farmabios S.p.A. IT	Triancinolona acetonido	18100213	1
Farmabios S.p.A./Cae...	Triancinolona acetonido	15233901	1
Fiebig	Triancinolona acetonido	15C19-B06-308571	1
Fiebig	Triancinolona acetonido	16B04-B07-318957	1
Fiebig	Triancinolona acetonido	17057902	1
Fiebig	Triancinolona acetonido	1805001-02	1
Fiebig	Triancinolona acetonido	20000461004	1
Finteler Apotheke	Triancinolona acetonido	17057910	1
fragon/phonix	Triancinolona acetonido	18K16-B05-357636	1
Fragon	Triancinolona acetonido	21H25-F03-379867	1
Fragron/ Alliance	Triancinolona acetonido	20L-18-F01-376658	1
Gehe amax	Triancinolona acetonido	17C09-B01-340174	1
Gehe amax	Triancinolona acetonido	1801020-01	1
Gehe amax	Triancinolona acetonido	1903015-01	1
Gehe Apo-ident	Triancinolona acetonido	201200601	1
Gehe Rostock	Triancinolona acetonido	19120211	1
Gehe Rostock	Triancinolona acetonido	21000116019	1
Gehe Rostock	Triancinolona acetonido	2100016019	1
Gehe/EuRo	Triancinolona acetonido	1605010-01	1
Gehe/EuRo	Triancinolona acetonido	1801020-01	1
Gehe/EuRoh	Triancinolona acetonido	2006002-01	1
Gehe/Fragon	Triancinolona acetonido	16D14-B11-325479	1
Gehe/Phönix	Triancinolona acetonido	1209040-02	1
Gehe	Triancinolona acetonido	12/10-N09	2
Gehe	Triancinolona acetonido	12301510	2
Gehe	Triancinolona acetonido	12E15-N03	1
Gehe	Triancinolona acetonido	13124805	1
Gehe	Triancinolona acetonido	13E15-N03	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Triancinolona acetonido	13I26-N11	1
Gehe	Triancinolona acetonido	1504007-01	1
Gehe	Triancinolona acetonido	15430102	2
Gehe	Triancinolona acetonido	15B02-B03-303827	1
GEHE	Triancinolona acetonido	1605010-01	1
Gehe	Triancinolona acetonido	160800501	1
Gehe	Triancinolona acetonido	1608005-01	1
Gehe	Triancinolona acetonido	16094501	1
Gehe	Triancinolona acetonido	1612014-01	1
GEHE	Triancinolona acetonido	16K07-B06-332103	1
Gehe	Triancinolona acetonido	1703037	1
Gehe	Triancinolona acetonido	170601301	1
Gehe	Triancinolona acetonido	1706013-01	2
GEHE	Triancinolona acetonido	1706013-01	1
Gehe	Triancinolona acetonido	1710002-01	1
GEHE	Triancinolona acetonido	1710002-01	1
Gehe	Triancinolona acetonido	17120606	2
Gehe	Triancinolona acetonido	17120610	1
GEHE	Triancinolona acetonido	17358303	1
Gehe	Triancinolona acetonido	1801020-01	1
Gehe	Triancinolona acetonido	1805001-01	1
Gehe	Triancinolona acetonido	1805001-02	1
Gehe	Triancinolona acetonido	1810015-01	2
GEHE	Triancinolona acetonido	1810015-01	1
Gehe	Triancinolona acetonido	18100203	1
Gehe	Triancinolona acetonido	18100206	1
GEHE	Triancinolona acetonido	18100206	1
Gehe	Triancinolona acetonido	18100208	2
Gehe	Triancinolona acetonido	18100222	1
GEHE	Triancinolona acetonido	18100225	2
Gehe	Triancinolona acetonido	18C15-B05	1
Gehe	Triancinolona acetonido	18K16-B05-367959	1
Gehe	Triancinolona acetonido	1903015-01	3
Gehe	Triancinolona acetonido	1903018-01	1
Gehe	Triancinolona acetonido	19J11-F02	1
Gehe	Triancinolona acetonido	20000461003	1
Gehe	Triancinolona acetonido	20000461004	1
Gehe	Triancinolona acetonido	2001017-01	1
Gehe	Triancinolona acetonido	2012006-01	1
Gehe	Triancinolona acetonido	20B28F04371542	1
Gehe	Triancinolona acetonido	21000116001	2
Gehe	Triancinolona acetonido	21000116005	1
Gehe	Triancinolona acetonido	21000116014	1
Gehe	Triancinolona acetonido	2109004-03	1
Gehe	Triancinolona acetonido	21H25-F03-379875	1
Gehe	Triancinolona acetonido	22000902005	1
GEHE	Triancinolona acetonido	22000902012	1
gehe	Triancinolona acetonido	22000902019	1
gehe	Triancinolona acetonido	2200902019	1
Gehe	Triancinolona acetonido	2208004-01	3
GEHE	Triancinolona acetonido	2208004-02	1
Gehe	Triancinolona acetonido	22A22-B01-218005	3
Gehe	Triancinolona acetonido	700124-0007	1
Geibo/ Fargron	Triancinolona acetonido	16D14-B11-322158	1
Geilenkirchen	Triancinolona acetonido	18K16-B05-357775	1
Geilenkirchen	Triancinolona acetonido	20000461007	1
Geilenkirchen	Triancinolona acetonido	21000116008	1
Hirsch	Triancinolona acetonido	12I10-N09	2
Ichtyol/Gehe	Triancinolona acetonido	15430102	3
Jenne	Triancinolona acetonido	1805001-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Triancinolona acetonido	18C15-B05-347275	1
Jenne	Triancinolona acetonido	2012006-01	1
Jenne	Triancinolona acetonido	21000116001	1
Jenne	Triancinolona acetonido	2109004-01	2
Jenne	Triancinolona acetonido	22000902019	2
Jenne	Triancinolona acetonido	2208004-01	1
Kehr	Triancinolona acetonido	1057902	1
Kehr	Triancinolona acetonido	21003093005	1
Kehr	Triancinolona acetonido	22000902005	1
Kehr	Triancinolona acetonido	22000902019	1
Kehr	Triancinolona acetonido	2200902014	1
Kehr	Triancinolona acetonido	22A22-B01-218005	1
Klenk	Triancinolona acetonido	1504007-02	1
Klenk	Triancinolona acetonido	NS1680M	1
Lamotte	Triancinolona acetonido	19120207	1
Martinus-Apotheke	Triancinolona acetonido	13379905	1
Midas Göttingen	Triancinolona acetonido	16094504	1
Midas	Triancinolona acetonido	16094511	1
Midas	Triancinolona acetonido	17H03-B12-343457	1
Newchem / Gehe	Triancinolona acetonido	18F14-B01-355979	1
Newchem / Gehe	Triancinolona acetonido	191202005	1
Newchem / Gehe	Triancinolona acetonido	B05-3598701	1
Newchem / Gehe	Triancinolona acetonido	NV2998M	1
NEWCHEM / Sanacorp	Triancinolona acetonido	15040007-01	1
Newchem S. p. A. / Noweda	Triancinolona acetonido	17120608	1
Newchem S.p.A./Caesa…	Triancinolona acetonido	1543015	1
NEWCHEM S.P.A.	Triancinolona acetonido	NV0994M	1
Newchem S.P.A/Allian…	Triancinolona acetonido	2006032-01	1
Newchem S.P.A	Triancinolona acetonido	1508008-02	1
Newchem Spa (site)	Triancinolona acetonido	16K07-B06-332102	1
Newchem Spa	Triancinolona acetonido	191202006	1
Newchem Spa	Triancinolona acetonido	19J11-F02-367962	1
Newchem/ Jenne	Triancinolona acetonido	18F14-B01-356853	1
Newchem/ Noweda	Triancinolona acetonido	1403009-01	1
Newchem/AHD	Triancinolona acetonido	1407044-02	1
Newchem/Fiebig	Triancinolona acetonido	1605010-01	1
Newchem/Kehr	Triancinolona acetonido	1407044-01	1
Newchem/Noweda	Triancinolona acetonido	15C19-B06-308573	1
Newchem/Noweda	Triancinolona acetonido	NA3551M	1
Newchem/Noweda	Triancinolona acetonido	NZ0071M	2
Newchem/Noweda	Triancinolona acetonido	NZ3279M	1
Newchem/Phönix	Triancinolona acetonido	1810015-01	1
Newchem	Triancinolona acetonido	1303001-02	1
Noveda	Triancinolona acetonido	12301518	1
Noweda/ NEWCHEM	Triancinolona acetonido	1211013-02	1
Noweda/Fargon	Triancinolona acetonido	18K16-B05-359868	1
Noweda	Triancinolona acetonido	1112023-02	1
Noweda	Triancinolona acetonido	12301501	1
Noweda	Triancinolona acetonido	12301509	1
Noweda	Triancinolona acetonido	12E15-N03	1
noweda	Triancinolona acetonido	13256604	1
Noweda	Triancinolona acetonido	13K15-B31-289029	1
Noweda	Triancinolona acetonido	1407044-01	1
Noweda	Triancinolona acetonido	14355103	1
Noweda	Triancinolona acetonido	14355708	1
Noweda	Triancinolona acetonido	15233902	1
Noweda	Triancinolona acetonido	15233903	1
Noweda	Triancinolona acetonido	1605010-01	1
Noweda	Triancinolona acetonido	1608005-01	1
Noweda	Triancinolona acetonido	16094514	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Triancinolona acetonido	1703037-01	4
Noweda	Triancinolona acetonido	17057905	2
Noweda	Triancinolona acetonido	17057908	1
Noweda	Triancinolona acetonido	1706013-01	1
Noweda	Triancinolona acetonido	17120603	1
Noweda	Triancinolona acetonido	17120606	2
Noweda	Triancinolona acetonido	17120611	1
Noweda	Triancinolona acetonido	17358305	2
Noweda	Triancinolona acetonido	17H03-B12-343457	1
Noweda	Triancinolona acetonido	1805001-01	1
Noweda	Triancinolona acetonido	181000226	1
Noweda	Triancinolona acetonido	1810015-01	2
Noweda	Triancinolona acetonido	18100210	2
Noweda	Triancinolona acetonido	18100213	1
Noweda	Triancinolona acetonido	18100221	1
Noweda	Triancinolona acetonido	18100222	2
Noweda	Triancinolona acetonido	18K16B05359867	1
Noweda	Triancinolona acetonido	1903015-01	1
Noweda	Triancinolona acetonido	1907044-01	1
Noweda	Triancinolona acetonido	191202005	1
Noweda	Triancinolona acetonido	19120211	1
Noweda	Triancinolona acetonido	2006032-01	1
Noweda	Triancinolona acetonido	2012006-01	1
Noweda	Triancinolona acetonido	21000116014	1
Noweda	Triancinolona acetonido	21000116022	1
Noweda	Triancinolona acetonido	21003093001	1
Noweda	Triancinolona acetonido	2109004-02	1
Noweda	Triancinolona acetonido	21H25-F03-379863	1
Noweda	Triancinolona acetonido	2200902018	1
Noweda	Triancinolona acetonido	2208004-01	4
Noweda	Triancinolona acetonido	F04-3715401	1
Noweda	Triancinolona acetonido	FO4-3715401	1
Noweda	Triancinolona acetonido	NZ1748M	1
Oberlinden Apotheke	Triancinolona acetonido	B0544/114010	1
Oberlinden- Apotheke	Triancinolona acetonido	U0544/113530	1
Oberlinden-Apotheke	Triancinolona acetonido	U0544/1	1
Parthe Apotheke	Triancinolona acetonido	55/21	1
Pharmachem/Phönix	Triancinolona acetonido	1907044-01	1
Phoenix /Eu Rho	Triancinolona acetonido	2006002-01	1
Phoenix 07.03.2017 11,62EUR	Triancinolona acetonido	16D14-B11-325480	1
Phoenix 12.03.2019 11,43EUR	Triancinolona acetonido	18F14-B01-352630	1
Phoenix WE 16.03.17 ...	Triancinolona acetonido	1612014-01	1
Phoenix,Eu Rho	Triancinolona acetonido	2208004-01	3
Phoenix	Triancinolona acetonido	13126-N11	2
Phoenix	Triancinolona acetonido	14355708	1
Phoenix	Triancinolona acetonido	14355709	1
Phoenix	Triancinolona acetonido	1703037	1
Phoenix	Triancinolona acetonido	1703037-01	1
Phoenix	Triancinolona acetonido	17057908	2
Phoenix	Triancinolona acetonido	1706013-01	4
Phoenix	Triancinolona acetonido	17120603	2
Phoenix	Triancinolona acetonido	1805001-01	1
Phoenix	Triancinolona acetonido	18100221	1
Phoenix	Triancinolona acetonido	2012006-01	1
Phoenix	Triancinolona acetonido	2012006-02	1
Phoenix	Triancinolona acetonido	2109004-02	1
Phoenix	Triancinolona acetonido	21H25-F03_379875	1
Phoenix	Triancinolona acetonido	22000902008	1
Phoenix	Triancinolona acetonido	22000902019	1
Phoenix	Triancinolona acetonido	3064	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Triancinolona acetonido	3129	1
Phoenix	Triancinolona acetonido	3219	1
Phoenix	Triancinolona acetonido	3424	1
Phoenix_25.01.2019	Triancinolona acetonido	1810015-01	2
phoenix-06.11.18	Triancinolona acetonido	1801020-01	1
Phönix Gotha	Triancinolona acetonido	14355711	1
Phönix Gotha	Triancinolona acetonido	17120610	1
Phönix Gotha	Triancinolona acetonido	191202005	1
Phönix W.E: 16.04.20...	Triancinolona acetonido	1710002-01	1
Phönix/Apo-Ident	Triancinolona acetonido	6702021007	1
Phönix/Caesar&Lorenz...	Triancinolona acetonido	21003093001	1
Phönix	Triancinolona acetonido	12E15-N03	1
Phönix	Triancinolona acetonido	13379902	1
Phönix	Triancinolona acetonido	13E15-N03	1
Phönix	Triancinolona acetonido	13K15-B31-289027	1
Phönix	Triancinolona acetonido	1403009-01	1
Phönix	Triancinolona acetonido	1407044-01	1
phönix	Triancinolona acetonido	15233906	1
phönix	Triancinolona acetonido	15430107	1
phönix	Triancinolona acetonido	1605010-01	1
Phönix	Triancinolona acetonido	1608005-01	1
Phönix	Triancinolona acetonido	17057908	2
Phönix	Triancinolona acetonido	1706013-01	1
Phönix	Triancinolona acetonido	1801020-01	1
Phönix	Triancinolona acetonido	1805001-02	1
Phönix	Triancinolona acetonido	1810015-01	2
Phönix	Triancinolona acetonido	18100204	1
Phönix	Triancinolona acetonido	18F14-B01-032343	1
Phönix	Triancinolona acetonido	18K16-B05-359871	2
Phönix	Triancinolona acetonido	18K16-B05-361521	1
Phönix	Triancinolona acetonido	1903015	1
Phönix	Triancinolona acetonido	1907044-01	1
Phönix	Triancinolona acetonido	19120207	1
Phönix	Triancinolona acetonido	19120209	1
Phönix	Triancinolona acetonido	19120210	1
Phönix	Triancinolona acetonido	19120211	2
Phönix	Triancinolona acetonido	20000461003	1
Phönix	Triancinolona acetonido	20002630001	1
Phönix	Triancinolona acetonido	20002630005	2
Phönix	Triancinolona acetonido	2001017-01	1
Phönix	Triancinolona acetonido	2006002-01	2
Phönix	Triancinolona acetonido	200850209	2
Phönix	Triancinolona acetonido	2012006-01	2
PHÖNIX	Triancinolona acetonido	21000116008	1
Phönix	Triancinolona acetonido	21000116011	1
Phönix	Triancinolona acetonido	22000902010	1
Phönix	Triancinolona acetonido	2208004-01	1
Phönix	Triancinolona acetonido	TAC7	1
Röntgen	Triancinolona acetonido	1903015-01	1
Sanacorp	Triancinolona acetonido		1
Sanacorp	Triancinolona acetonido	100/AKD4	1
Sanacorp	Triancinolona acetonido	12301506	1
Sanacorp	Triancinolona acetonido	13124807	2
Sanacorp	Triancinolona acetonido	1326N11	1
Sanacorp	Triancinolona acetonido	13379905	1
Sanacorp	Triancinolona acetonido	13E15-N03	1
sanacorp	Triancinolona acetonido	15233902	1
Sanacorp	Triancinolona acetonido	15430108	1
Sanacorp	Triancinolona acetonido	1710002-01	1
Sanacorp	Triancinolona acetonido	17120605	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Triancinolona acetonido	17120610	1
Sanacorp	Triancinolona acetonido	17358302	1
Sanacorp	Triancinolona acetonido	17358305	1
Sanacorp	Triancinolona acetonido	17H03-B12-345553	1
Sanacorp	Triancinolona acetonido	18100220	1
Sanacorp	Triancinolona acetonido	18100221	3
Sanacorp	Triancinolona acetonido	18fB01355724	1
Sanacorp	Triancinolona acetonido	18K16-B05-359867	1
Sanacorp	Triancinolona acetonido	191202005	1
Sanacorp	Triancinolona acetonido	19120208	3
Sanacorp	Triancinolona acetonido	19120209	1
Sanacorp	Triancinolona acetonido	2006002-01	1
Sanacorp	Triancinolona acetonido	20B28-F04-371546	1
Sanacorp	Triancinolona acetonido	20L18-F01-376658	1
Sanacorp	Triancinolona acetonido	210001604	1
Sanacorp	Triancinolona acetonido	2100309093004	1
Sanacorp	Triancinolona acetonido	2109004-02	1
Sanacorp	Triancinolona acetonido	21H25-F03-379874	1
Sanacorp	Triancinolona acetonido	22000902002	1
Sanacorp	Triancinolona acetonido	2208004-01	1
Sanacorp	Triancinolona acetonido	2208004-02	1
Sanacorp	Triancinolona acetonido	22A22-B01-218005	1
Sanacorp	Triancinolona acetonido	22D15-B01-222391	1
Sanacorp	Triancinolona acetonido	2308018-01	1
Sanacorp	Triancinolona acetonido	NY0485M	2
Schulzendorfer Apotheke	Triancinolona acetonido	2208004-02	1
Sittig	Triancinolona acetonido	1508008-02	1
Spangro 15.1.2014	Triancinolona acetonido	1303001-02	1
Spangro 27.03.18	Triancinolona acetonido	17030337-01	1
Spangropharm	Triancinolona acetonido	1209040-02	1
Tiarnyao/Gehe	Triancinolona acetonido	2001017-01	1
VDL	Triancinolona acetonido	13379903	1
WE: 08.12.2015	Triancinolona acetonido	14K14-B05-302887	1

- 230 508 spectra from 1515 *Apo-Ident* customers from a total of 48 428 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triancinolona acetonido* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triancinolona acetonido* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	722	0	152 240
Type B	0	1679	0	200 405
Type C	0	5501	58	230 508

The substance/substance group *Triancinolona acetonido* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1690 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6426 %)
Type C	100.0000 % (> 99.9007 %)	98.9566 % (> 98.9027 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20765	20765	0,00	80,12
20910	21061	4,05	79,40
21061	21061	0,00	77,19
21072	21061	4,09	79,24
21587	21587	0,00	79,55
21883	21883	0,00	76,70
21962	21587	14,35	80,92
22313	22313	0,00	76,44
22572	22572	0,00	80,51
22752	22752	0,00	74,14
25339	25339	0,00	159,24
25560	25560	0,00	78,33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triclosan**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20005-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triclosan; Triclosanum

Special notes

When selecting the *Triclosan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triclosan	8	17	695

Second-stage model

For differentiation of the substance/substance group *Triclosan* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triclosan* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cloridrato de oxitetraciclina	104,95	–
⋮	⋮	⋮
Citrato de sódio	>50	211,15
Capsaicina	>50	284,44
Metoxisaleno	>50	328,57
Cloridrato de quinina di-hidratado	>50	409,51
Levocarnitina	>50	425,49
Heparina sódica	>50	451,76
Cloridrato de oxibutinina	>50	462,70
Prednicarbato	>50	563,12
Piridoxal-5-fosfato	>50	568,52
Cloridrato de ciprofloxacina	>50	668,27
Tetracaína	>50	837,62
Alfaestradiol	>50	842,79
Acetato de ciproterona	>50	950,56
Amifampridina	>50	977,62
Sacarose	>50	1015,40
Acetato de noretisterona	>50	1731,38
Cloridrato de amitriptilina	>50	2031,07
Valina	>50	2840,26

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triclosan* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triclosan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triclosan	13391808	21509	60	20131211
Caelo	Triclosan	14121209	21591	45	20140718

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triclosan	1406032-01	21615	60	20140710
Euro OTC	Triclosan	1507041	21856	60	20150804*
Euro OTC	Triclosan	1510045	22227	60	20150511*
Euro OTC	Triclosan	1602003	22373	45	20160204*
Euro OTC	Triclosan	1701032	22987	40	20170207*
Fagron	Triclosan	17K02-B06-343548	23915	40	20180105

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 8 reference samples from the substance/substance group *Triclosan*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 552 spectra from a total of 2834 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 20 reference samples from the substance/substance group *Triclosan*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triclosan	160846	22453	60
Caelo	Triclosan	162808	22775	40
Caelo	Triclosan	171498	23315	40
Caelo	Triclosan	180814	24048	40
Caelo	Triclosan	182537	24387	40
Caelo	Triclosan	192709	25221	40
Caelo	Triclosan	23002009	27331	40
Euro OTC	Triclosan	1607002	22674	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Triclosan	1705011	23425	40
Euro OTC	Triclosan	1708025	23699	40
Euro OTC	Triclosan	1801049	23964	40
Euro OTC	Triclosan	1901006	24466	40
Euro OTC	Triclosan	1912002	24927	40
Euro OTC	Triclosan	2001027	25097	40
Euro OTC	Triclosan	2101029	25578	40
Euro OTC	Triclosan	2206016	26217	40
Fagron	Triclosan	21B25-B02-203360	26284	40
Caelo	Triclosan	23002009	27331SI	20
Euro OTC	Triclosan	2206016	26217SI	20
Fagron	Triclosan	21B25-B02-203360	26284SI	20

- 201 324 spectra from a total of 4028 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6465 spectra from 1263 *Apo-Ident* customers from 732 batches from the substance/substance group *Triclosan*.

- Among them are spectra of independent samples from 676 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Triclosan		1
	Triclosan	/20/11/6107	1
	Triclosan	20J30-B03-204649	1
	Triclosan	21000427001	2
	Triclosan	21000427002	2
	Triclosan	21000427003	3
	Triclosan	21000427005	4
	Triclosan	21000427006	4
	Triclosan	21000427007	1
	Triclosan	21000427008	4
	Triclosan	21000427009	3
	Triclosan	21000427010	1
	Triclosan	21000427011	14
	Triclosan	21000427014	14
	Triclosan	21000427015	8
	Triclosan	21000427016	3
	Triclosan	21000427017	7
	Triclosan	21000428015	1
	Triclosan	21000428016	1
	Triclosan	21000428017	3
	Triclosan	21000428020	9
	Triclosan	21000428021	3
	Triclosan	21000428022	5
	Triclosan	2100427011	1
	Triclosan	2101029-02	2
	Triclosan	2101029-04	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Triclosan	21B25-B02-203359	1
	Triclosan	21B25-B02-203363	1
	Triclosan	21B25-B02-203393	1
	Triclosan	220601601	1
	Triclosan	2206016-01	15
	Triclosan	220601602	1
	Triclosan	2206016-02	9
	Triclosan	2206016-03	2
	Triclosan	2208016-02	1
	Triclosan	23002009001	8
	Triclosan	23002009003	2
18253716	Triclosan		1
30.01.2019 Phoenix	Triclosan	18081415	1
73681 Indien / Gehe	Triclosan	1912002-01	1
73681 Indien / Gehe	Triclosan	1912002-03	1
A.H.D.	Triclosan	12L06-N01	1
AEP	Triclosan	18253722	1
agron/ Noweda	Triclosan	13A11-N03	1
AHC 02.09.13 EK9,04	Triclosan	13D02-N02	1
AHD 17.01.15	Triclosan	13L18-B35-289992	1
AHD	Triclosan	17081723	1
AHD	Triclosan	18081417	2
AHD	Triclosan	18253705	1
AHD	Triclosan	21000427006	1
AHD	Triclosan	21000427007	1
AHD	Triclosan	21000427008	1
AHD	Triclosan	21000427009	2
AHD	Triclosan	21000427017	1
AHD	Triclosan	21000428021	1
AHL	Triclosan	1801049-01	2
ALH	Triclosan	1607002-01	2
Alliance Health 26.1...	Triclosan	13L18-B35-289995	1
Alliance Healthcare/...	Triclosan	13H09-N01	1
Alliance Healthcare	Triclosan	12G09-N09	1
Alliance Healthcare	Triclosan	12L06-N01	1
Alliance Healthcare	Triclosan	13D02-N02	1
Alliance Healthcare	Triclosan	13L-18-835	1
Alliance Healthcare	Triclosan	16084608	1
Alliance/EuRho	Triclosan	1912002-03	3
Alliance	Triclosan	1912002-003	1
Alliance	Triclosan	192709018	1
Alliance	Triclosan	21000427008	1
Alliance	Triclosan	21000427011	1
Alliance	Triclosan	21000428005	1
alliance	Triclosan	21000428022	2
Alliance	Triclosan	2101029-02	1
Alliance	Triclosan	23002009003	2
Allianz	Triclosan	1801049-01	1
anzag 20.11.2013	Triclosan	12359114	1
Anzag 4.12.12 ek:8,89	Triclosan	12G17-N04	1
Anzag	Triclosan	12G09-N09	2
Anzag	Triclosan	12G17-N04	3
Anzag	Triclosan	13L18-B35-289995	1
Anzag	Triclosan	1607002-01	2
Anzag	Triclosan	1701032-02	1
Anzag	Triclosan	192709015	1
Anzag	Triclosan	192709022	1
Anzag	Triclosan	2100427015	1
Anzag	Triclosan	5846205	1
Anzag06.	Triclosan	14F23-B02-295758	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
apo-ident	Triclosan	1708025-01	1
apomix	Triclosan	1406032-01	2
apomix	Triclosan	14F23-B02-295760	1
apomix	Triclosan	17149813	1
Apotheke an der Born...	Triclosan	16280817	3
Audor Pharma	Triclosan		2
BASF Chem trade GmbH...	Triclosan	5846205	1
BASF Grenzach GmbH/Phönix	Triclosan	10006226	1
BASF Grenzach GmbH/Phönix	Triclosan	13A11-N03	1
BASF Grenzach GmbH/Phönix	Triclosan	13A11-No3	1
BASF Grenzach GmbH/Phönix	Triclosan	13D02-N02	1
BASF Grenzach GmbH/Phönix	Triclosan	13H09-N01	1
BASF Grenzach/Noweda	Triclosan	5900346	1
BASF	Triclosan	1505009-01	1
BASF	Triclosan	1708025-01	1
Beiersdorf	Triclosan	14F23-B02-295764	1
Bionorica/Phönix	Triclosan	1708025-01	1
Bombastus	Triclosan	12359111	1
Bombastus	Triclosan	12L06-N01	2
Bombastus	Triclosan	13L18-35-289984	1
Bombastus	Triclosan	1408024-01	1
Bombastus	Triclosan	14f23-b02-300219	1
Bombastus	Triclosan	17081726	1
Bombastus	Triclosan	17149809	1
Caeclo/Phönix	Triclosan	1705011-01	2
Cael	Triclosan	182537002	1
Caeleo/ Kehr	Triclosan	192709025	1
Caelo	Triclosan		5
Caelo	Triclosan	10206240	1
Caelo	Triclosan	108144416	1
Caelo	Triclosan	11076716	1
Caelo	Triclosan	11076717	2
Caelo	Triclosan	11238003	2
Caelo	Triclosan	11238004	1
Caelo	Triclosan	11238009	2
Caelo	Triclosan	11238011	1
Caelo	Triclosan	1125204	1
Caelo	Triclosan	1149806	1
Caelo	Triclosan	11777748	3
Caelo	Triclosan	12003201	3
Caelo	Triclosan	12003202	1
Caelo	Triclosan	12003205	7
Caelo	Triclosan	12003210	5
Caelo	Triclosan	12145901	5
Caelo	Triclosan	12145902	5
Caelo	Triclosan	12145906	6
Caelo	Triclosan	12145907	9
Caelo	Triclosan	12145908	7
Caelo	Triclosan	12145909	11
Caelo	Triclosan	12145910	11
Caelo	Triclosan	12145917	1
Caelo	Triclosan	12276827	1
Caelo	Triclosan	12359104	6
Caelo	Triclosan	12359105	7
Caelo	Triclosan	12359106	11
Caelo	Triclosan	12359107	1
Caelo	Triclosan	12359108	13
Caelo	Triclosan	12359109	3
Caelo	Triclosan	12359110	5
Caelo	Triclosan	12359111	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	12359112	8
Caelo	Triclosan	12359114	1
Caelo	Triclosan	12537002	1
Caelo	Triclosan	12680801	1
Caelo	Triclosan	1280801	1
Caelo	Triclosan	12c21-n05	1
Caelo	Triclosan	12G17-N04	2
Caelo	Triclosan	12106-n01	1
Caelo	Triclosan	12L06-N01	7
Caelo	Triclosan	12L06-N01/0005900346	1
Caelo	Triclosan	13247805	1
Caelo	Triclosan	13247903	1
Caelo	Triclosan	13247904	11
Caelo	Triclosan	13247905	10
Caelo	Triclosan	13247908	2
Caelo	Triclosan	13391801	2
Caelo	Triclosan	13391802	4
Caelo	Triclosan	13391804	10
Caelo	Triclosan	13391807	3
Caelo	Triclosan	13391808	9
Caelo	Triclosan	13A11-N03	2
Caelo	Triclosan	13D02-N02	7
Caelo	Triclosan	13D02-No2	1
Caelo	Triclosan	13H08-N10	2
Caelo	Triclosan	13H09-N01	7
Caelo	Triclosan	13L18-B35-289984	1
Caelo	Triclosan	13L18B35289986	1
Caelo	Triclosan	13L18-B35-289986	2
Caelo	Triclosan	13L18-B35-289987	1
Caelo	Triclosan	13L18-B35-289992	2
Caelo	Triclosan	13L18B35289993	1
Caelo	Triclosan	13L18-B35-289995	1
Caelo	Triclosan	14052101	5
Caelo	Triclosan	14052102	11
Caelo	Triclosan	14052103	14
Caelo	Triclosan	14052105	1
Caelo	Triclosan	1412109	1
Caelo	Triclosan	14121203	10
Caelo	Triclosan	14121204	9
Caelo	Triclosan	14121207	10
Caelo	Triclosan	14121209	6
Caelo	Triclosan	14121210	11
Caelo	Triclosan	14121211	9
Caelo	Triclosan	14121214	13
Caelo	Triclosan	14121215	14
Caelo	Triclosan	14121220	1
Caelo	Triclosan	1418E-03402	1
Caelo	Triclosan	14205901	7
Caelo	Triclosan	14205902	9
Caelo	Triclosan	14205903	15
Caelo	Triclosan	14205904	6
Caelo	Triclosan	14205905	6
Caelo	Triclosan	14211207	1
Caelo	Triclosan	14211211	1
Caelo	Triclosan	14F23-B02	1
Caelo	Triclosan	14F23B02293859	1
Caelo	Triclosan	14F23-B02-295758	1
Caelo	Triclosan	14F23-B02-295760	1
Caelo	Triclosan	14F23-B02-295765	1
Caelo	Triclosan	150103201	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1501032-02	1
Caelo	Triclosan	1503603	1
Caelo	Triclosan	1505009	1
Caelo	Triclosan	150704101	1
Caelo	Triclosan	1507041-01	2
Caelo	Triclosan	15121202	1
Caelo	Triclosan	15203603	14
Caelo	Triclosan	15203604	14
Caelo	Triclosan	15203606	9
Caelo	Triclosan	15203607	15
Caelo	Triclosan	15203608	11
Caelo	Triclosan	1520603	1
Caelo	Triclosan	1530105	1
Caelo	Triclosan	15301501	1
Caelo	Triclosan	15301502	13
Caelo	Triclosan	15301503	12
Caelo	Triclosan	15301504	12
Caelo	Triclosan	15301505	12
Caelo	Triclosan	15301506	18
Caelo	Triclosan	15301510	2
Caelo	Triclosan	15301511	9
Caelo	Triclosan	15301512	6
Caelo	Triclosan	15301513	1
Caelo	Triclosan	15301514	1
Caelo	Triclosan	15c10-b06	1
Caelo	Triclosan	15C10-B06-310031	3
Caelo	Triclosan	15C10-B06-310031	1
Caelo	Triclosan	15C10-B06-311161	1
Caelo	Triclosan	15C10-B06-312982	3
Caelo	Triclosan	15G07-B03-30039	1
Caelo	Triclosan	15G07-B03-310035	1
Caelo	Triclosan	15G07-B03-310035/201	1
Caelo	Triclosan	15G07-B03-310037	2
Caelo	Triclosan	15G07-B03-310038	2
Caelo	Triclosan	15G07-B03-310040	1
Caelo	Triclosan	160084601	1
Caelo	Triclosan	1602003-01	2
Caelo	Triclosan	16021306	1
Caelo	Triclosan	160280811	1
Caelo	Triclosan	16064616	1
Caelo	Triclosan	1607002-01	2
Caelo	Triclosan	16071801	1
Caelo	Triclosan	160846	1
Caelo	Triclosan	16084601	7
Caelo	Triclosan	160846018	1
Caelo	Triclosan	16084602	10
Caelo	Triclosan	16084603	15
Caelo	Triclosan	16084606	5
Caelo	Triclosan	16084607	11
Caelo	Triclosan	16084608	17
Caelo	Triclosan	16084609	3
Caelo	Triclosan	16084610	11
Caelo	Triclosan	16084611	17
Caelo	Triclosan	16084614	20
Caelo	Triclosan	16084617	1
Caelo	Triclosan	16084618	16
Caelo	Triclosan	16084620	1
Caelo	Triclosan	16084621	1
Caelo	Triclosan	16084622	1
Caelo	Triclosan	1609005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1609005-02	2
Caelo	Triclosan	1620809	1
Caelo	Triclosan	16253716	1
Caelo	Triclosan	162808	1
Caelo	Triclosan	16280801	29
Caelo	Triclosan	16280802	23
Caelo	Triclosan	16280802-30417/1	1
Caelo	Triclosan	16280803	5
Caelo	Triclosan	16280805	2
Caelo	Triclosan	16280808	21
Caelo	Triclosan	16280809	8
Caelo	Triclosan	16280810	1
Caelo	Triclosan	16280811	19
Caelo	Triclosan	16280816	17
Caelo	Triclosan	16280817	14
Caelo	Triclosan	16280818	7
Caelo	Triclosan	16280819	7
Caelo	Triclosan	1628082	1
Caelo	Triclosan	16280820	13
Caelo	Triclosan	16280821	2
Caelo	Triclosan	16280824	4
Caelo	Triclosan	16280874	1
Caelo	Triclosan	162820817	1
Caelo	Triclosan	16293901	1
Caelo	Triclosan	1701032	1
Caelo	Triclosan	1701032-01	3
Caelo	Triclosan	170501101	2
Caelo	Triclosan	1705011-01	7
Caelo	Triclosan	170802-01	1
Caelo	Triclosan	170802501	1
Caelo	Triclosan	1708025-01	4
Caelo	Triclosan	170817	1
Caelo	Triclosan	17081702	1
Caelo	Triclosan	17081703	11
Caelo	Triclosan	17081704	1
Caelo	Triclosan	17081705	12
Caelo	Triclosan	17081706	4
Caelo	Triclosan	17081707	26
Caelo	Triclosan	170817075274	1
Caelo	Triclosan	17081709	20
Caelo	Triclosan	17081710	19
Caelo	Triclosan	17081711	17
Caelo	Triclosan	17081712	18
Caelo	Triclosan	17081713	9
Caelo	Triclosan	17081714	12
Caelo	Triclosan	17081716	17
Caelo	Triclosan	17081716-T20180112Ma	1
Caelo	Triclosan	17081717	8
Caelo	Triclosan	17081720	31
Caelo	Triclosan	17081721	24
Caelo	Triclosan	17081722	30
Caelo	Triclosan	17081723	10
Caelo	Triclosan	17081724	23
Caelo	Triclosan	17081725	19
Caelo	Triclosan	17081726	16
Caelo	Triclosan	170817265507	1
Caelo	Triclosan	1708173	1
Caelo	Triclosan	170919Di	1
Caelo	Triclosan	171449809	1
Caelo	Triclosan	1714819	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	17148927	1
Caelo	Triclosan	1714926	1
Caelo	Triclosan	1714930	1
Caelo	Triclosan	17149621	1
Caelo	Triclosan	171498	1
Caelo	Triclosan	17149801	5
Caelo	Triclosan	17149805	10
Caelo	Triclosan	17149806	13
Caelo	Triclosan	17149807	17
Caelo	Triclosan	17149808	40
Caelo	Triclosan	171498085598	1
Caelo	Triclosan	17149809	50
Caelo	Triclosan	17149810P-190531-3	1
Caelo	Triclosan	17149812	16
Caelo	Triclosan	17149812-20180619Ma4	1
Caelo	Triclosan	17149813	19
Caelo	Triclosan	17149813-T20181115Ma	1
Caelo	Triclosan	17149814	20
Caelo	Triclosan	17149815	14
Caelo	Triclosan	17149817	6
Caelo	Triclosan	17149818	1
Caelo	Triclosan	17149819	32
Caelo	Triclosan	17149820	20
Caelo	Triclosan	17149821	39
Caelo	Triclosan	17149822	15
Caelo	Triclosan	17149824	9
Caelo	Triclosan	17149825	26
Caelo	Triclosan	17149826	1
Caelo	Triclosan	17149827	22
Caelo	Triclosan	171499808	1
Caelo	Triclosan	171499815	1
Caelo	Triclosan	171549805	1
Caelo	Triclosan	1719809	1
Caelo	Triclosan	1719814	1
Caelo	Triclosan	1748912	1
Caelo	Triclosan	1749825	1
Caelo	Triclosan	17801712	1
Caelo	Triclosan	1781720	1
Caelo	Triclosan	17K02-B06_343544	2
Caelo	Triclosan	17K02-B06-343543	1
Caelo	Triclosan	180081408	1
Caelo	Triclosan	1801417	1
Caelo	Triclosan	18061407	1
Caelo	Triclosan	180811401	1
Caelo	Triclosan	18081401	8
Caelo	Triclosan	18081402	21
Caelo	Triclosan	18081403	15
Caelo	Triclosan	18081405	43
Caelo	Triclosan	18081406	33
Caelo	Triclosan	18081407	37
Caelo	Triclosan	18081408	55
Caelo	Triclosan	18081409	1
Caelo	Triclosan	18081410	14
Caelo	Triclosan	18081411	1
Caelo	Triclosan	18081413	39
Caelo	Triclosan	18081414	30
Caelo	Triclosan	18081415	42
Caelo	Triclosan	18081416	37
Caelo	Triclosan	18081417	50
Caelo	Triclosan	1808414	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	18243726	1
Caelo	Triclosan	18253/06	1
Caelo	Triclosan	18253078	1
Caelo	Triclosan	182533722	1
Caelo	Triclosan	182537001	61
Caelo	Triclosan	182537002	51
Caelo	Triclosan	18253701	6
Caelo	Triclosan	18253702	12
Caelo	Triclosan	18253703	3
Caelo	Triclosan	18253705	47
Caelo	Triclosan	182537052	1
Caelo	Triclosan	18253706	41
Caelo	Triclosan	18253707	38
Caelo	Triclosan	18253708	42
Caelo	Triclosan	18253709	32
Caelo	Triclosan	18253710	8
Caelo	Triclosan	18253711	33
Caelo	Triclosan	18253712	28
Caelo	Triclosan	18253713P-200116-1	1
Caelo	Triclosan	18253714	11
Caelo	Triclosan	18253715	3
Caelo	Triclosan	18253716	57
Caelo	Triclosan	18253717	19
Caelo	Triclosan	18253718	22
Caelo	Triclosan	18253721	30
Caelo	Triclosan	18253722	35
Caelo	Triclosan	18253724	6
Caelo	Triclosan	182537247	1
Caelo	Triclosan	18253726	17
Caelo	Triclosan	18253729	1
Caelo	Triclosan	18253731	2
Caelo	Triclosan	1825717	1
Caelo	Triclosan	182597001	1
Caelo	Triclosan	185237002	1
Caelo	Triclosan	18523716	1
Caelo	Triclosan	1852537001	1
Caelo	Triclosan	185253711	1
Caelo	Triclosan	1901006-01	1
Caelo	Triclosan	1901006-02	1
Caelo	Triclosan	1901006-03	1
Caelo	Triclosan	190709021	1
Caelo	Triclosan	1912002-01	1
Caelo	Triclosan	1912002-03	3
Caelo	Triclosan	192109015	1
Caelo	Triclosan	1922709021	1
Caelo	Triclosan	1927009013	1
Caelo	Triclosan	192708022	1
Caelo	Triclosan	192709002	24
Caelo	Triclosan	192709003	10
Caelo	Triclosan	192709004	18
Caelo	Triclosan	192709006	1
Caelo	Triclosan	192709007	11
Caelo	Triclosan	192709008	1
Caelo	Triclosan	192709009	8
Caelo	Triclosan	192709010	16
Caelo	Triclosan	192709011	30
Caelo	Triclosan	192709012	34
Caelo	Triclosan	192709013	20
Caelo	Triclosan	192709014	34
Caelo	Triclosan	192709014/4720	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	192709015	31
Caelo	Triclosan	192709016	32
Caelo	Triclosan	192709018	8
Caelo	Triclosan	192709020	41
Caelo	Triclosan	192709021	49
Caelo	Triclosan	192709022	32
Caelo	Triclosan	192709023	14
Caelo	Triclosan	192709025	31
Caelo	Triclosan	19270913	1
Caelo	Triclosan	1927099021	1
Caelo	Triclosan	19709007	1
Caelo	Triclosan	2000428001	1
Caelo	Triclosan	20021304	1
Caelo	Triclosan	200701407	1
Caelo	Triclosan	200870409	1
Caelo	Triclosan	21000427	1
Caelo	Triclosan	21000427001	13
Caelo	Triclosan	21000427002	6
Caelo	Triclosan	21000427005	4
Caelo	Triclosan	21000427006	2
Caelo	Triclosan	21000427007	11
Caelo	Triclosan	21000427008	1
Caelo	Triclosan	21000427009	1
Caelo	Triclosan	21000427011	3
Caelo	Triclosan	21000427017	1
Caelo	Triclosan	21000428001	33
Caelo	Triclosan	21000428002	1
Caelo	Triclosan	21000428003	23
Caelo	Triclosan	21000428004	21
Caelo	Triclosan	21000428005	7
Caelo	Triclosan	21000428008	24
Caelo	Triclosan	21000428009	23
Caelo	Triclosan	2100042801	1
Caelo	Triclosan	21000428010	21
Caelo	Triclosan	21000428011	17
Caelo	Triclosan	21000428012	13
Caelo	Triclosan	21000428013	7
Caelo	Triclosan	21000428015	16
Caelo	Triclosan	21000428016	16
Caelo	Triclosan	21000428017	10
Caelo	Triclosan	21000428021	11
Caelo	Triclosan	2100042812	1
Caelo	Triclosan	21000828001	1
Caelo	Triclosan	2100427001	1
Caelo	Triclosan	2100428001	4
Caelo	Triclosan	2100428011	1
Caelo	Triclosan	228711-514	1
Caelo	Triclosan	23121409	1
Caelo	Triclosan	2317I-03402	1
Caelo	Triclosan	28011	1
Caelo	Triclosan	3041408	1
Caelo	Triclosan	39(192709020)	1
Caelo	Triclosan	5012E-03402	1
Caelo	Triclosan	517E-03402	1
Caelo	Triclosan	5203607	1
Caelo	Triclosan	6121711	1
Caelo	Triclosan	8081401	1
Caelo	Triclosan	8253718	1
Caelo	Triclosan	87767	1
Caelo	Triclosan	AKD12	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	bhfdd	1
Caelo	Triclosan	Caelo	2
Caeo/Noweda	Triclosan	15301505	1
Caeo/Sanacorp	Triclosan	18081405	1
Caeolo/Noweda	Triclosan	13247905	1
Caeolo/Phönix	Triclosan	18081416	1
Caeolo	Triclosan	17149809	1
Caesar & Lorenz GmbH	Triclosan	192709016	1
Caesar & Lorenz	Triclosan	21000428020	1
Caesar & Loretz GmbH…	Triclosan	18253721	1
Caesar & Loretz GmbH…	Triclosan	21000428015	1
Caesar & Loretz GmbH…	Triclosan	182537001	1
Caesar & Loretz GmbH…	Triclosan	18253708	1
Caesar & Loretz GmbH…	Triclosan	18253717	1
Caesar & Loretz GmbH…	Triclosan	21000427011	2
Caesar & Loretz GmbH…	Triclosan	192709015	2
Caesar & Loretz GmbH…	Triclosan	192709016	2
Caesar & Loretz GmbH…	Triclosan	17149813	1
Caesar & Loretz GmbH…	Triclosan	18081413	2
Caesar & Loretz GmbH…	Triclosan	18081416	1
Caesar & Loretz GmbH…	Triclosan	21000427001	2
Caesar & Loretz GmbH…	Triclosan	18253705	1
Caesar & Loretz GmbH…	Triclosan	18253730	1
Caesar & Loretz GmbH…	Triclosan	18081417	1
Caesar & Loretz GmbH…	Triclosan	18253709	2
Caesar & Loretz GmbH…	Triclosan	18253710	1
Caesar & Loretz GmbH…	Triclosan	18253707	1
Caesar & Loretz GmbH/ AHD	Triclosan	18081416	1
Caesar & Loretz GmbH…	Triclosan	192709016	2
Caesar & Loretz GmbH…	Triclosan	21000428008	1
Caesar & Loretz GmbH…	Triclosan	192709022	2
Caesar & Loretz GmbH…	Triclosan	192709020	2
Caesar & Loretz GmbH…	Triclosan	21000427003	1
Caesar & Loretz GmbH…	Triclosan	192709022	1
Caesar & Loretz GmbH/AHD	Triclosan	192709011	1
Caesar & Loretz GmbH/AHD	Triclosan	21000428021	2
Caesar & Loretz GmbH…	Triclosan	192709020	2
Caesar & Loretz GmbH…	Triclosan	18081408	1
Caesar & Loretz GmbH…	Triclosan	18081417	1
Caesar & Loretz GmbH…	Triclosan	192709016	1
Caesar & Loretz GmbH…	Triclosan	192709021	1
Caesar & Loretz GmbH…	Triclosan	21000428011	1
Caesar & Loretz GmbH/Gehe	Triclosan	18253708	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709012	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709013	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709014	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709016	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709025	1
Caesar & Loretz GmbH/Gehe	Triclosan	21000427002	1
Caesar & Loretz GmbH/Gehe	Triclosan	21000428010	1
Caesar & Loretz GmbH/Gehe	Triclosan	21000428011	2
Caesar & Loretz GmbH…	Triclosan	18253707	1
Caesar & Loretz GmbH…	Triclosan	192709002	1
Caesar & Loretz GmbH…	Triclosan	192709009	1
Caesar & Loretz GmbH…	Triclosan	192709012	1
Caesar & Loretz GmbH…	Triclosan	192709022	1
Caesar & Loretz GmbH…	Triclosan	21000428001	1
Caesar & Loretz GmbH…	Triclosan	21000428009	1
Caesar & Loretz GmbH…	Triclosan	21000428010	1
Caesar & Loretz GmbH…	Triclosan	21000428011	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Triclosan	AP210406-01	1
Caesar & Loretz GmbH/Kehr	Triclosan	18253707	1
Caesar & Loretz GmbH/Kehr	Triclosan	18253712	1
Caesar & Loretz GmbH/Kehr	Triclosan	18253721	1
Caesar & Loretz GmbH/Kehr	Triclosan	192709014	1
Caesar & Loretz GmbH/Kehr	Triclosan	21000427002	1
Caesar & Loretz GmbH/Kehr	Triclosan	21000428003	1
Caesar & Loretz GmbH...	Triclosan	18081413	1
Caesar & Loretz GmbH...	Triclosan	18253721	1
Caesar & Loretz GmbH...	Triclosan	18253708	1
Caesar & Loretz GmbH...	Triclosan	18081407	1
Caesar & Loretz GmbH...	Triclosan	182537002	1
Caesar & Loretz GmbH...	Triclosan	18253711	3
Caesar & Loretz GmbH...	Triclosan	192709003	1
Caesar & Loretz GmbH...	Triclosan	192709007	2
Caesar & Loretz GmbH...	Triclosan	192709018	4
Caesar & Loretz GmbH...	Triclosan	192709020	2
Caesar & Loretz GmbH...	Triclosan	21000428004	1
Caesar & Loretz GmbH...	Triclosan	21000428015	2
Caesar & Loretz GmbH...	Triclosan	21000428017	1
Caesar & Loretz GmbH...	Triclosan	21000427007	2
Caesar & Loretz GmbH...	Triclosan	21000428003	1
Caesar & Loretz GmbH...	Triclosan	21000428010	1
Caesar & Loretz GmbH...	Triclosan	18253718	4
Caesar & Loretz GmbH...	Triclosan	18253712	1
Caesar & Loretz GmbH...	Triclosan	182537002	4
Caesar & Loretz GmbH...	Triclosan	18253706	1
Caesar & Loretz GmbH...	Triclosan	18253714	1
Caesar & Loretz GmbH...	Triclosan	18253722	1
Caesar & Loretz GmbH...	Triclosan	192709016	1
Caesar & Loretz GmbH...	Triclosan	192709021	1
Caesar & Loretz GmbH...	Triclosan	192709025	2
Caesar & Loretz GmbH...	Triclosan	21000427001	1
Caesar & Loretz GmbH...	Triclosan	21000428001	2
Caesar & Loretz GmbH...	Triclosan	21000428003	1
Caesar & Loretz GmbH...	Triclosan	21000428005	1
Caesar & Loretz GmbH...	Triclosan	21000428011	1
Caesar & Loretz GmbH...	Triclosan	18253711	1
Caesar & Loretz GmbH...	Triclosan	18253721	2
Caesar & Loretz GmbH...	Triclosan	18253722	1
Caesar & Loretz GmbH...	Triclosan	192709011	1
Caesar & Loretz GmbH...	Triclosan	192709013	2
Caesar & Loretz GmbH...	Triclosan	192709021	1
Caesar & Loretz GmbH...	Triclosan	192709021	1
Caesar & Loretz GmbH...	Triclosan	21000428009	3
Caesar & Loretz GmbH...	Triclosan	21000428012	2
Caesar & Loretz GmbH...	Triclosan	21000428015	1
Caesar & Loretz GmbH...	Triclosan	21000428017	1
Caesar & Loretz GmbH	Triclosan	15081416	1
Caesar & Loretz GmbH	Triclosan	1609005-01	1
Caesar & Loretz GmbH	Triclosan	16280811	1
Caesar & Loretz GmbH	Triclosan	17149806	1
Caesar & Loretz GmbH	Triclosan	17149813	1
Caesar & Loretz GmbH	Triclosan	17149821	1
Caesar & Loretz GmbH	Triclosan	18081403	1
Caesar & Loretz GmbH	Triclosan	18081410	1
Caesar & Loretz GmbH	Triclosan	18081413	1
Caesar & Loretz GmbH	Triclosan	18081414	3
Caesar & Loretz GmbH	Triclosan	18081416	4
Caesar & Loretz GmbH	Triclosan	18081417	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Triclosan	182537001	13
Caesar & Loretz GmbH	Triclosan	182537002	9
Caesar & Loretz GmbH	Triclosan	18253702	2
Caesar & Loretz GmbH	Triclosan	18253705	9
Caesar & Loretz GmbH	Triclosan	18253706	13
Caesar & Loretz GmbH	Triclosan	18253707	5
Caesar & Loretz GmbH	Triclosan	18253708	5
Caesar & Loretz GmbH	Triclosan	18253709	9
Caesar & Loretz GmbH	Triclosan	18253710	6
Caesar & Loretz GmbH	Triclosan	18253711	3
Caesar & Loretz GmbH	Triclosan	18253712	4
Caesar & Loretz GmbH	Triclosan	18253714	2
Caesar & Loretz GmbH	Triclosan	18253716	19
Caesar & Loretz GmbH	Triclosan	18253717	4
Caesar & Loretz GmbH	Triclosan	18253718	7
Caesar & Loretz GmbH	Triclosan	18253721	5
Caesar & Loretz GmbH	Triclosan	18253722	2
Caesar & Loretz GmbH	Triclosan	18253724	2
Caesar & Loretz GmbH	Triclosan	18253726	6
Caesar & Loretz GmbH	Triclosan	190100602	1
Caesar & Loretz GmbH	Triclosan	1912002-01	1
Caesar & Loretz GmbH	Triclosan	1912002-04	1
Caesar & Loretz GmbH	Triclosan	192709002	6
Caesar & Loretz GmbH	Triclosan	192709003	1
Caesar & Loretz GmbH	Triclosan	192709004	3
Caesar & Loretz GmbH	Triclosan	192709009	1
Caesar & Loretz GmbH	Triclosan	192709010	2
Caesar & Loretz GmbH	Triclosan	192709011	7
Caesar & Loretz GmbH	Triclosan	192709012	6
Caesar & Loretz GmbH	Triclosan	192709013	9
Caesar & Loretz GmbH	Triclosan	192709014	5
Caesar & Loretz GmbH	Triclosan	192709015	12
Caesar & Loretz GmbH	Triclosan	192709016	8
Caesar & Loretz GmbH	Triclosan	192709018	5
Caesar & Loretz GmbH	Triclosan	192709020	14
Caesar & Loretz GmbH	Triclosan	192709021	21
Caesar & Loretz GmbH	Triclosan	192709022	13
Caesar & Loretz GmbH	Triclosan	192709023	3
Caesar & Loretz GmbH	Triclosan	192709024	1
Caesar & Loretz GmbH	Triclosan	192709025	5
Caesar & Loretz GmbH	Triclosan	19279003	2
Caesar & Loretz GmbH	Triclosan	20003964012	1
Caesar & Loretz GmbH	Triclosan	2001027-01	1
Caesar & Loretz GmbH	Triclosan	21000427001	7
Caesar & Loretz GmbH	Triclosan	21000427003	2
Caesar & Loretz GmbH	Triclosan	21000427005	1
Caesar & Loretz GmbH	Triclosan	21000427007	4
Caesar & Loretz GmbH	Triclosan	21000427008	1
Caesar & Loretz GmbH	Triclosan	21000427011	2
Caesar & Loretz GmbH	Triclosan	21000428001	9
Caesar & Loretz GmbH	Triclosan	21000428003	8
Caesar & Loretz GmbH	Triclosan	21000428004	4
Caesar & Loretz GmbH	Triclosan	21000428005	1
Caesar & Loretz GmbH	Triclosan	21000428008	8
Caesar & Loretz GmbH	Triclosan	21000428009	6
Caesar & Loretz GmbH	Triclosan	21000428010	7
Caesar & Loretz GmbH	Triclosan	21000428011	13
Caesar & Loretz GmbH	Triclosan	21000428012	7
Caesar & Loretz GmbH	Triclosan	21000428013	4
Caesar & Loretz GmbH	Triclosan	21000428015	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Triclosan	21000428016	4
Caesar & Loretz GmbH	Triclosan	21000428017	4
Caesar & Loretz GmbH	Triclosan	21000428018	1
Caesar & Loretz GmbH	Triclosan	21000428021	4
Caesar & Loretz GmbH	Triclosan	AP210205-02	1
Caesar & Loretz Hild…	Triclosan	192709013	1
Caesar & Loretz Hilden	Triclosan	18081408	1
Caesar & Loretz Hilden	Triclosan	18081413	1
Caesar & Loretz Hilden	Triclosan	18081414	1
Caesar & Loretz Hilden	Triclosan	18081417	2
Caesar & Loretz Hilden	Triclosan	182537001	2
Caesar & Loretz Hilden	Triclosan	18253707	1
Caesar & Loretz Hilden	Triclosan	18253709	1
Caesar & Loretz Hilden	Triclosan	18253710	1
Caesar & Loretz Hilden	Triclosan	18253717	1
Caesar & Loretz Hilden	Triclosan	18253726	1
Caesar & Loretz Hilden	Triclosan	192709002	1
Caesar & Loretz Hilden	Triclosan	192709011	1
Caesar & Loretz/ Noweda	Triclosan	17149812	1
Caesar & Loretz/AHC	Triclosan	16084603	2
Caesar & Loretz/AHD	Triclosan	14121209	1
Caesar & Loretz	Triclosan	17081705	1
Caesar / Ebert	Triclosan	17081716	1
Caesar / Gehe	Triclosan	18253709	1
Caesar u Loretz	Triclosan	15301503	1
Caesar und Loretz GmbH	Triclosan	17149808	1
Caesar und Loretz	Triclosan	15301502	1
Caesar&Lorenz / Gehe	Triclosan	18253716	1
Caesar&Lorenz / Gehe	Triclosan	18253722	1
Caesar&Lorenz	Triclosan	17081707	1
Caesar&Lorenz	Triclosan	21000428001	1
Caesar&Lorenz	Triclosan	21000428010	1
Caesar&Loretz GmbH/Anzag	Triclosan	14121215	2
Caesar&Loretz GmbH/Anzag	Triclosan	15203603	2
Caesar&Loretz GmbH/S…	Triclosan	15301505	1
Caesar&Loretz GmbH	Triclosan	16084609	1
Caesar&Loretz GmbH	Triclosan	16280808	1
Caesar&Loretz GmbH	Triclosan	192709002	1
Caesar&Loretz GmbH	Triclosan	192709025	1
Caesar&Loretz,AHC,12…	Triclosan	16084618	1
Caesar&loretz,Phönix	Triclosan	15203606	1
caesar&loretz,Phönix	Triclosan	15203607	1
Caesar/Lorenz	Triclosan	12145910	1
Caesar/Lorenz	Triclosan	12359104	1
Caesar/Lorenz	Triclosan	13247904	1
Caleo/Phönix	Triclosan	17081711	1
Carlo/Phönix/23,50	Triclosan	1901006-01	1
Cealo/AHD	Triclosan	14F23-B02-295947	1
Cealo/Anzag	Triclosan	182537002	1
Cealo/Gehe	Triclosan	17149807	1
Cealo/Phoenix	Triclosan	192709015	1
Cealo/Sanacorp	Triclosan	192709025	1
Cealo	Triclosan	16280801	1
Cealo	Triclosan	17081723	1
Cealo	Triclosan	17149809	1
Cealo	Triclosan	18081403	1
Cealo	Triclosan	18081405	1
Cealo	Triclosan	18081416	1
Cealo	Triclosan	192709016	1
Cealo	Triclosan	21000428003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo	Triclosan	71215/1Gie	1
Celo/Phonix	Triclosan	16084611	1
Crystal pharma/ Ober…	Triclosan	15203603	1
DAB 2008	Triclosan	12003201	2
Delta Apotheke	Triclosan	17149822	1
E Plus	Triclosan	16280808	1
E Plus	Triclosan	17081705	1
Easy Höchst	Triclosan	17149822	1
ebe a	Triclosan	14121207	1
Eigenproduktion	Triclosan	13A11-N03	1
EuRho / 30	Triclosan	1401038-01	1
EuRho / fiebig	Triclosan	1705011-01	1
EuRho / Fiebig	Triclosan	2001027	1
EuRho /11	Triclosan	1912002-01	1
EuRho Gehe	Triclosan	1801049-01	1
EuRho GEHE	Triclosan	1912002-01	2
EuRho/ Phoenix	Triclosan	2101029-01	1
Eurho/A	Triclosan	2101029-01	2
eurho/AHC	Triclosan	2001027-01	1
EuRho/Gehe	Triclosan	1912002-02	1
EuRho/Gehe	Triclosan	2001027-01	1
EuRho/Noweda	Triclosan	1708025-01	2
EuRho/Noweda	Triclosan	1901006-03	1
EuRho/Phoenix	Triclosan	1401038-01	1
EuRho/Phönix	Triclosan	1307050-01	2
EuRho/Phönix	Triclosan	1912002-01	1
EuRho/Phönix	Triclosan	1912002-02	1
Eurho/Phönix	Triclosan	210102901	1
Eurho/S	Triclosan	2101029-02	1
Eurho/Sanacorp	Triclosan	2101029-01	1
EuRho	Triclosan	1107030-01	2
EuRho	Triclosan	1202018-01	1
EuRho	Triclosan	1206034-02	2
EuRho	Triclosan	1408024-01	1
EuRho	Triclosan	151004501	1
EuRho	Triclosan	1705011-01	1
EuRho	Triclosan	1708025-01	1
EuRho	Triclosan	1901006-01	1
EuRho	Triclosan	1901006-02	4
EuRho	Triclosan	1901006-03	1
EuRho	Triclosan	1912002-01	1
euRho	Triclosan	191200204	1
EuRho	Triclosan	2101029-01	1
Eurho	Triclosan	2101029-02	1
EuRho	Triclosan	2101029-02	3
EuRho	Triclosan	k0011	1
EuRhoNoweda	Triclosan	1602003-01	1
Euro OCT/Noweda	Triclosan	1501032-02	1
Euro OCT	Triclosan	1912002-01	1
Euro OTC	Triclosan		13
Euro OTC	Triclosan	/19/07/3301	1
Euro OTC	Triclosan	/20/11/6107	2
Euro OTC	Triclosan	1107030-01	3
Euro OTC	Triclosan	1202018-01	1
Euro OTC	Triclosan	1202018-02	2
Euro OTC	Triclosan	120203-02	1
Euro OTC	Triclosan	1206034-01	1
Euro OTC	Triclosan	120603402	1
Euro OTC	Triclosan	1206034-02	3
Euro OTC	Triclosan	1211025-01	11

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	12276023	2
Euro OTC	Triclosan	12276024	1
Euro OTC	Triclosan	12276027	3
Euro OTC	Triclosan	12276028	5
Euro OTC	Triclosan	1245	1
Euro OTC	Triclosan	130301101	1
Euro OTC	Triclosan	1303011-01	5
Euro OTC	Triclosan	1307050-01	6
Euro OTC	Triclosan	13247904	1
Euro OTC	Triclosan	13H08-N10	1
Euro OTC	Triclosan	140103801	1
Euro OTC	Triclosan	1401038-01	10
Euro OTC	Triclosan	140603201	1
Euro OTC	Triclosan	1406032-01	10
Euro OTC	Triclosan	1408024-01	6
Euro OTC	Triclosan	14121204	1
Euro OTC	Triclosan	14F23-B02-295948	1
Euro OTC	Triclosan	1501032-01	10
Euro OTC	Triclosan	1501032-02	4
Euro OTC	Triclosan	150500901	1
Euro OTC	Triclosan	1505009-01	12
Euro OTC	Triclosan	15058946	2
Euro OTC	Triclosan	1507041-01	7
Euro OTC	Triclosan	151004501	1
Euro OTC	Triclosan	1510045-01	19
Euro OTC	Triclosan	15150229	2
Euro OTC	Triclosan	15203607	3
Euro OTC	Triclosan	1550229	1
Euro OTC	Triclosan	15C10-B06-312981	1
Euro OTC	Triclosan	15C10-B06-312982	1
Euro OTC	Triclosan	15G07-B03-310036	1
Euro OTC	Triclosan	15G07-B03-310040	1
Euro OTC	Triclosan	1602003	2
Euro OTC	Triclosan	160200301	1
Euro OTC	Triclosan	1602003-01	29
Euro OTC	Triclosan	16047002-01	1
Euro OTC	Triclosan	160531T	1
Euro OTC	Triclosan	160700201	1
Euro OTC	Triclosan	1607002-01	34
Euro OTC	Triclosan	160702-01	1
Euro OTC	Triclosan	16084614	1
Euro OTC	Triclosan	160900-02	1
Euro OTC	Triclosan	16090005-02	1
Euro OTC	Triclosan	1609005-01	30
Euro OTC	Triclosan	160900502	1
Euro OTC	Triclosan	1609005-02	27
Euro OTC	Triclosan	16280820	1
Euro OTC	Triclosan	169005-02	1
Euro OTC	Triclosan	1701032	1
Euro OTC	Triclosan	1701032_01	1
Euro OTC	Triclosan	1701032-01	17
Euro OTC	Triclosan	170103202	1
Euro OTC	Triclosan	1701032-02	16
Euro OTC	Triclosan	1701037-01	1
Euro OTC	Triclosan	170113T1609005-01	1
Euro OTC	Triclosan	170132-01	1
Euro OTC	Triclosan	170501101	2
Euro OTC	Triclosan	1705011-01	48
Euro OTC	Triclosan	170511-01	1
Euro OTC	Triclosan	170511-010012276028	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	170526T/1701032-02	1
Euro OTC	Triclosan	17080-01	1
Euro OTC	Triclosan	1708025	1
Euro OTC	Triclosan	1708025_01	1
Euro OTC	Triclosan	170802501	2
Euro OTC	Triclosan	1708025-01	47
Euro OTC	Triclosan	1708025-01P-181001-3	1
Euro OTC	Triclosan	1708025-01P181129-4	1
Euro OTC	Triclosan	17081703	1
Euro OTC	Triclosan	17081722	1
Euro OTC	Triclosan	170825-01	1
Euro OTC	Triclosan	171121T/1705011-01	1
Euro OTC	Triclosan	17149806	1
Euro OTC	Triclosan	17149808	1
Euro OTC	Triclosan	17149812	1
Euro OTC	Triclosan	17149815	1
Euro OTC	Triclosan	17K02-B06-343548	2
Euro OTC	Triclosan	1801049	1
Euro OTC	Triclosan	1801049-01	12
Euro OTC	Triclosan	1801049-21	1
Euro OTC	Triclosan	180149-01	1
Euro OTC	Triclosan	1805001-01	1
Euro OTC	Triclosan	18253706	2
Euro OTC	Triclosan	1901006	1
Euro OTC	Triclosan	1901006-002	1
Euro OTC	Triclosan	190100601	2
Euro OTC	Triclosan	1901006-01	58
Euro OTC	Triclosan	190100602	2
Euro OTC	Triclosan	1901006-02	33
Euro OTC	Triclosan	1901006-03	17
Euro OTC	Triclosan	1901006-1	3
Euro OTC	Triclosan	1901006-1P-190506-2	1
Euro OTC	Triclosan	191006-02	1
Euro OTC	Triclosan	19120002-02	1
Euro OTC	Triclosan	19120003	1
Euro OTC	Triclosan	1912001-01	1
Euro OTC	Triclosan	1912002	3
Euro OTC	Triclosan	1912002-001	1
Euro OTC	Triclosan	191200201	4
Euro OTC	Triclosan	1912002-01	46
Euro OTC	Triclosan	1912002-02	19
Euro OTC	Triclosan	191200203	2
Euro OTC	Triclosan	1912002-03	40
Euro OTC	Triclosan	1912002-04	21
Euro OTC	Triclosan	19122002-03	1
Euro OTC	Triclosan	20001027-01	1
Euro OTC	Triclosan	2001027-01	28
Euro OTC	Triclosan	2101025-01	1
Euro OTC	Triclosan	2101029	2
Euro OTC	Triclosan	210102901	1
Euro OTC	Triclosan	2101029-01	46
Euro OTC	Triclosan	2101029-02	19
Euro OTC	Triclosan	2101029-03	7
Euro OTC	Triclosan	21011029-02	1
Euro OTC	Triclosan	2206016-01	12
Euro OTC	Triclosan	2206016-02	1
Euro OTC	Triclosan	3078439	1
Euro OTC	Triclosan	4486611	2
Euro OTC	Triclosan	5860088	1
Euro OTC	Triclosan	700228	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	CHB1303011-01	1
Euro OTC	Triclosan	K/00111809334	1
Euro UTC	Triclosan	1510045-01	1
Euro/Anzag	Triclosan	1607002-01	1
Euro/Gehe	Triclosan	1602003-01	1
Euro/Noweda	Triclosan	1607002-01	1
Euro/Phoenix	Triclosan	1912002-04	1
Euro/Phoenix	Triclosan	2101029-01	2
Euro/Phönix	Triclosan	160900502	1
Euro/Phönix	Triclosan	170103201	1
Euro/Phönix	Triclosan	1901006	2
Euro/Phönix	Triclosan	1912002-02	1
Euro/Sanacorp	Triclosan	1701032-01	1
Euro/Sanacorp	Triclosan	1912002-01	1
Euro	Triclosan	2001027-01	1
Euroct/Gehe	Triclosan	1510045-01	2
EuRoh/ Gehe	Triclosan	17149821	1
EuRoh/ Gehe	Triclosan	1901006-02	1
EuRoh/ Gehe	Triclosan	191200202	1
EuRoh	Triclosan		1
Euroo/direkt	Triclosan	1705011-01	1
Europ Ots Pharma	Triclosan	13DO2-NO2	1
EurRho/Gehe	Triclosan		1
EurRho/Noweda	Triclosan	1912002-04	1
Fagro/Gehe	Triclosan	13H08-N10	1
Fagro/Sanacorp	Triclosan	TCS0214037	1
Fagron	Triclosan		5
Fagron	Triclosan	10006226	2
Fagron	Triclosan	1006226	1
Fagron	Triclosan	10112014C	1
Fagron	Triclosan	10666066	2
Fagron	Triclosan	106666066	1
Fagron	Triclosan	10J18-N01	2
Fagron	Triclosan	11238004	1
Fagron	Triclosan	11777748	4
Fagron	Triclosan	11A05-N13	2
Fagron	Triclosan	11c21-n05	1
Fagron	Triclosan	11D20-N10	1
Fagron	Triclosan	11h09-n02	1
Fagron	Triclosan	11H09-N02	6
Fagron	Triclosan	11J28-n02	1
Fagron	Triclosan	11J28-N02	4
Fagron	Triclosan	11L19-N11	7
Fagron	Triclosan	1209213402	1
Fagron	Triclosan	1214I03402	1
Fagron	Triclosan	12c21-n05	3
Fagron	Triclosan	12C21-N05	23
Fagron	Triclosan	12G09-N09	4
Fagron	Triclosan	12G09-no9	1
Fagron	Triclosan	12g17-n04	2
Fagron	Triclosan	12G17-n04	2
Fagron	Triclosan	12G17N04	1
Fagron	Triclosan	12G17-N04	30
Fagron	Triclosan	12l06-n01	1
Fagron	Triclosan	12L06-n01	1
Fagron	Triclosan	12L06-N01	35
Fagron	Triclosan	13092012C	1
Fagron	Triclosan	13a11n03	1
Fagron	Triclosan	13A11N03	1
Fagron	Triclosan	13A11-N03	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	13A11-NO3	1
Fagron	Triclosan	13C10-B06-312981	1
Fagron	Triclosan	13d02-n02	1
Fagron	Triclosan	13d02-N02	1
Fagron	Triclosan	13D02N02	1
Fagron	Triclosan	13D02-N02	66
Fagron	Triclosan	13D02-N-02	1
Fagron	Triclosan	13Do2-N02	1
Fagron	Triclosan	13DO2-NO2	1
Fagron	Triclosan	13h08-n10	1
Fagron	Triclosan	13H08N10	2
Fagron	Triclosan	13H08-N10	30
Fagron	Triclosan	13H08-N-10	1
Fagron	Triclosan	13H08-N100450/1231	1
Fagron	Triclosan	13h09-n01	1
Fagron	Triclosan	13H09N01	2
Fagron	Triclosan	13H09-N01	60
Fagron	Triclosan	13H09-N011296/2856	1
Fagron	Triclosan	13H09-No1	1
Fagron	Triclosan	13L18-35-289995	1
Fagron	Triclosan	13L18-B35	12
Fagron	Triclosan	13L18-B35_289995	1
Fagron	Triclosan	13L18-B35-289	1
Fagron	Triclosan	13L18-B35-289983	10
Fagron	Triclosan	13l18-b35-289984	1
Fagron	Triclosan	13L18B35289984	1
Fagron	Triclosan	13L18-B35-289984	5
Fagron	Triclosan	13L18-B35-289985	12
Fagron	Triclosan	13L18-B35-289985	1
Fagron	Triclosan	13L-18-B35-289985	1
Fagron	Triclosan	13L18-B35-289986	5
Fagron	Triclosan	13L18B35289987	1
Fagron	Triclosan	13L18-B35-289987	6
Fagron	Triclosan	13L18-B35-289988	1
Fagron	Triclosan	13L18-B35-289992	2
Fagron	Triclosan	13L18-B35-289993	4
Fagron	Triclosan	13l18-b35-289994	1
Fagron	Triclosan	13L18-B35-289994	7
Fagron	Triclosan	13L18-B35-289995	8
Fagron	Triclosan	14022014C	1
Fagron	Triclosan	14F23-B02	5
Fagron	Triclosan	14F23-B02_295756	1
Fagron	Triclosan	14F23-B02-293852	2
Fagron	Triclosan	14F23-B02-295756	2
Fagron	Triclosan	14f23-b02-295757	1
Fagron	Triclosan	14F23-B02295757	1
Fagron	Triclosan	14F23-B02-295757	6
Fagron	Triclosan	14f23-b02-295758	3
Fagron	Triclosan	14F23B02295758	1
Fagron	Triclosan	14F23-B02-295758	12
Fagron	Triclosan	14F23-B02-295759	9
Fagron	Triclosan	14F23-B02-295760	10
Fagron	Triclosan	14F23-B02-295761	11
Fagron	Triclosan	14F23-B02-295762	3
Fagron	Triclosan	14F23B02295763	1
Fagron	Triclosan	14F23-B02-295763	3
Fagron	Triclosan	14F23-B02-295764	2
Fagron	Triclosan	14F23-B02-295765	6
Fagron	Triclosan	14F23-B02-295947	6
Fagron	Triclosan	14F23-B02-295948	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	14F23-B02-2959947	1
Fagron	Triclosan	14F23B02300219	1
Fagron	Triclosan	14F23-B02-300219	7
Fagron	Triclosan	14F23-Bo2-295947	1
Fagron	Triclosan	14F-B02-293859	1
Fagron	Triclosan	151010-B06-312984	1
Fagron	Triclosan	15203604	1
Fagron	Triclosan	15301510	1
Fagron	Triclosan	15607-B03-310035	1
Fagron	Triclosan	15C10-806-312981	1
Fagron	Triclosan	15C10-B03-312982	1
Fagron	Triclosan	15C10-B06	5
Fagron	Triclosan	15C10-B06_312980	1
Fagron	Triclosan	15C10B06310031	2
Fagron	Triclosan	15C10-B06-310031	7
Fagron	Triclosan	15C10-B06-310032	4
Fagron	Triclosan	15c10-B06-311161	1
Fagron	Triclosan	15C10B06311161	2
Fagron	Triclosan	15C10-B06-311161	13
Fagron	Triclosan	15c10-b06-312980	1
Fagron	Triclosan	15c10-B06-312980	1
Fagron	Triclosan	15C10-B06-312980	6
Fagron	Triclosan	15c10-b06-312981	1
Fagron	Triclosan	15c10-B06-312981	1
Fagron	Triclosan	15C10-B06-312981	27
Fagron	Triclosan	15C10B06312982	1
Fagron	Triclosan	15C10-B06-312982	14
Fagron	Triclosan	15C10B06312983	1
Fagron	Triclosan	15C10-B06-312983	7
Fagron	Triclosan	15C10-B06-3161	1
Fagron	Triclosan	15C-B06-312982	1
Fagron	Triclosan	15G01-B03-310038	1
Fagron	Triclosan	15G047-B03-0001	1
Fagron	Triclosan	15G07	1
Fagron	Triclosan	15G07-B03	3
Fagron	Triclosan	15G07-B03_310037	1
Fagron	Triclosan	15G07-B03-30037	1
Fagron	Triclosan	15g07-b03-310035	1
Fagron	Triclosan	15G07-B03-310035	9
Fagron	Triclosan	15G07-B03-310036	4
Fagron	Triclosan	15G07B03310037	1
Fagron	Triclosan	15G07-B03-310037	13
Fagron	Triclosan	15G07-B03-310038	6
Fagron	Triclosan	15G07-B03-310039	3
Fagron	Triclosan	15G07B03310040	1
Fagron	Triclosan	15G07-B03-310040	6
Fagron	Triclosan	15G07-B03-310041	1
Fagron	Triclosan	160614	1
Fagron	Triclosan	16084603	1
Fagron	Triclosan	16084614	1
Fagron	Triclosan	1609005-02	2
Fagron	Triclosan	1708025-01	3
Fagron	Triclosan	17081702	1
Fagron	Triclosan	1710025	9
Fagron	Triclosan	17148812	1
Fagron	Triclosan	17149808	1
Fagron	Triclosan	17149814	3
Fagron	Triclosan	17149815	1
Fagron	Triclosan	17149817	2
Fagron	Triclosan	17149819	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	17G07-B03-310038	1
Fagron	Triclosan	17K02	1
Fagron	Triclosan	17K02-B06	8
Fagron	Triclosan	17K02-B06-343543	2
Fagron	Triclosan	17K02-B06-343544	10
Fagron	Triclosan	17K02-B06-343545	2
Fagron	Triclosan	17K02-B06343546	1
Fagron	Triclosan	17K02-B06-343546	15
Fagron	Triclosan	17K02-B06-343547	7
Fagron	Triclosan	17K02-B06-343548	9
Fagron	Triclosan	17K02-B06-34547	1
Fagron	Triclosan	18081414	1
Fagron	Triclosan	18082014B	1
Fagron	Triclosan	18253706	2
Fagron	Triclosan	1901006-01	1
Fagron	Triclosan	190282002	1
Fagron	Triclosan	190615A	1
Fagron	Triclosan	1912002-01	1
Fagron	Triclosan	1912002-02	2
Fagron	Triclosan	200315B	1
Fagron	Triclosan	20J30-B03	1
Fagron	Triclosan	20J30-B03-2046408	1
Fagron	Triclosan	20J30-B03-204647	1
Fagron	Triclosan	20J30-B03-204648	1
Fagron	Triclosan	20J30-B03-204649	1
Fagron	Triclosan	20J30-B03-2046-49	1
Fagron	Triclosan	21B25-B02	1
Fagron	Triclosan	21b25-b02-203393	1
Fagron	Triclosan	21B25-B02-203393	2
Fagron	Triclosan	220601601	1
Fagron	Triclosan	22B15-B05-218336	1
Fagron	Triclosan	2513Q-03402	1
Fagron	Triclosan	2901313402	1
Fagron	Triclosan	2914E-03402	1
Fagron	Triclosan	434083	1
Fagron	Triclosan	4394083	1
Fagron	Triclosan	4516I-03402	1
Fagron	Triclosan	5846205	2
Fagron	Triclosan	6012014E	1
Fagron	Triclosan	700228-0005	1
Fagron	Triclosan	90000383	1
Fagron	Triclosan	9000383	2
Fagron	Triclosan	B03-2046409	1
Fagron	Triclosan	C12H7Cl302	1
Fagron	Triclosan	KOO1-1/14/12/823	1
Fagron	Triclosan	TCS0214037	2
Fargon/Fönix	Triclosan	17081725	2
Fargon/Fönix	Triclosan	170817285	1
Fargon/Noweda	Triclosan	18081414	1
Fargon	Triclosan	12C21-N05	1
fargon	Triclosan	12G17-N04	1
Fargon	Triclosan	13D02-N02	2
Fargon	Triclosan	14F23-B02-295948	1
Fargon	Triclosan	4394403	1
Faron	Triclosan	14F23-B02-300219	2
Fiebig	Triclosan	15C10-B06-312923	1
Fiebig	Triclosan	1607002-01	1
Fiebig	Triclosan	16280811	1
Fiebig	Triclosan	17149813	1
Fiebig	Triclosan	17149814	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Triclosan	17149819	1
Fiebig	Triclosan	17149821	1
Fiebig	Triclosan	18081413	2
Fischar/Gehe	Triclosan	13D02-N02	1
Fragron	Triclosan	13D02-N02	1
Fragron	Triclosan	15G07-B03-310040	1
Gaesar & Loretz GmbH	Triclosan	21000427001	2
Gatt-Koller	Triclosan	21J01875	1
GEHE 17.06.2014	Triclosan	14052102	1
GEHE 22.04.2014	Triclosan	13391804	1
Gehe amax	Triclosan	15301503	1
Gehe/Fragon	Triclosan	15C10B06312981	2
Gehe	Triclosan		1
Gehe	Triclosan	11J28-N02	1
Gehe	Triclosan	12145910	1
Gehe	Triclosan	12359104	1
Gehe	Triclosan	12359105	1
Gehe	Triclosan	12359112	1
Gehe	Triclosan	12359114	1
Gehe	Triclosan	12l06-n01	1
Gehe	Triclosan	13391804	2
Gehe	Triclosan	13391811	1
Gehe	Triclosan	13A11-N03	1
Gehe	Triclosan	13D02-N02	1
Gehe	Triclosan	13L18-B35-289992	1
Gehe	Triclosan	14052105	1
Gehe	Triclosan	1408024-01	2
Gehe	Triclosan	14121210	1
Gehe	Triclosan	14121211	1
Gehe	Triclosan	14205904	1
Gehe	Triclosan	14F23B02295947	1
Gehe	Triclosan	14F23-B02-295947	1
Gehe	Triclosan	1505009-01	1
Gehe	Triclosan	16084614	1
Gehe	Triclosan	16280801	2
Gehe	Triclosan	16280808	1
Gehe	Triclosan	16280811	1
Gehe	Triclosan	1701032-01	1
GEHE	Triclosan	1701032-01	1
Gehe	Triclosan	1701032-02	1
GEHE	Triclosan	1701032-02	1
Gehe	Triclosan	1705011-01	1
Gehe	Triclosan	17081710	1
GEHE	Triclosan	17081710	1
Gehe	Triclosan	17149806	1
Gehe	Triclosan	17149809	1
Gehe	Triclosan	17149816	1
Gehe	Triclosan	17149820	2
GEHE	Triclosan	17149824	1
Gehe	Triclosan	18081408	1
Gehe	Triclosan	18253706	1
Gehe	Triclosan	18253709	1
Gehe	Triclosan	18253716	1
GEHE	Triclosan	18253724	1
Gehe	Triclosan	1901006-01	4
Gehe	Triclosan	190100602	1
Gehe	Triclosan	1912002-02	3
gehe	Triclosan	1912002-03	1
Gehe	Triclosan	1912002-03	1
Gehe	Triclosan	2001027-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Triclosan	21000427003	1
GEHE	Triclosan	21000427014	2
Gehe	Triclosan	21000427016	1
Gehe	Triclosan	21000427017	1
Gehe	Triclosan	21000428009	1
gehe	Triclosan	210102901	1
Gehe	Triclosan	2101029-01	3
Gehe	Triclosan	2101029-02	1
Gehe	Triclosan	22060016-01	1
Gehe	Triclosan	2206016-02	1
gehe	Triclosan	23002009001	4
Gehe	Triclosan	Caelo	2
Gehe-Fragon	Triclosan	14F23B02300219	2
Gehe-Fragon	Triclosan	15G07B03310036	2
Geilenkirchen	Triclosan	18253707	1
Geilenkirchen	Triclosan	18253711	1
Geilenkirchen	Triclosan	192709012	1
Gutenberg-Apotheke	Triclosan	13H09-N01	2
Gutenberg-Apotheke	Triclosan	13L18-B35	1
Henry Lamotte/ Noweda	Triclosan	15203606	1
Ichtyhol Gesellschaf…	Triclosan	1701032-02	1
Jenne	Triclosan	18081417	3
Jenne	Triclosan	1912002-03	1
Jenne	Triclosan	20J30-B03	2
Jenne	Triclosan	21000427014	3
Jenne	Triclosan	21000428010	2
Jiangsu EqualChem Co…	Triclosan	1710025	1
Kehr.09.07.2020	Triclosan	2001027-01	1
Kehr	Triclosan	21000427005	1
Kehr	Triclosan	21000427011	3
Kehr	Triclosan	21000427017	3
Kehr	Triclosan	2206016-01	1
Klenk	Triclosan	192709023	1
Klenk	Triclosan	21000428010	1
Klosterring	Triclosan	18081405	1
Kremer/Phönix	Triclosan	15/157/T	1
Krieger/Euro	Triclosan	2101029-01	1
Krieger	Triclosan	12g17-N04	1
Krieger	Triclosan	2206016-01	1
Kumar Organic Produc…	Triclosan	182537001	1
Kumar Organic Products	Triclosan	192709023	1
Kumar Organic/Noweda	Triclosan	15C10-B06	1
Kumar/Noweda	Triclosan		1
Kumar/Noweda	Triclosan	K0011/19/07/337	1
Kumar/Phoenix	Triclosan		2
L12	Triclosan	16280819	1
L12	Triclosan	1628081917181722	1
L12	Triclosan	18081408	1
L30/Alliance	Triclosan	1607002-01	1
Midas	Triclosan	17081714	2
Midas	Triclosan	17081721	1
Midas	Triclosan	17149815	1
Midas	Triclosan	17149819	1
Mvda_23.01.2019	Triclosan	18081416	1
Nachprüfung	Triclosan	AP200710-04	1
Nov	Triclosan	192709011	1
Noveda	Triclosan	18253707	1
now	Triclosan	18257001	1
Nowed 18.12.2014	Triclosan	14121210	2
Noweda 06.12.2019	Triclosan	18253721	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda 15.7.17	Triclosan	16280817	1
Noweda/EuRo	Triclosan	1801049-01	1
Noweda	Triclosan	12359107	1
Noweda	Triclosan	12G17-N04	2
Noweda	Triclosan	13247903	1
noweda	Triclosan	13L18-B35-289985	1
Noweda	Triclosan	1408024-01	1
Noweda	Triclosan	14F23-B02-295765	1
Noweda	Triclosan	15203603	2
Noweda	Triclosan	15203604	1
Noweda	Triclosan	16280818	1
Noweda	Triclosan	1705011-01	1
Noweda	Triclosan	17081703	1
Noweda	Triclosan	17081710	1
Noweda	Triclosan	17081711	1
Noweda	Triclosan	17081714	1
Noweda	Triclosan	17081721	1
Noweda	Triclosan	17081724	1
Noweda	Triclosan	17149801	1
Noweda	Triclosan	17149805	1
Noweda	Triclosan	17149815	1
Noweda	Triclosan	17K02-B06	1
Noweda	Triclosan	17K02-B06-343547	2
Noweda	Triclosan	18081413	1
Noweda	Triclosan	18081417	1
Noweda	Triclosan	182537002	1
Noweda	Triclosan	18253705	1
Noweda	Triclosan	18253708	2
Noweda	Triclosan	18253716	2
Noweda	Triclosan	18253717	1
Noweda	Triclosan	1912002-01	2
Noweda	Triclosan	192709007	1
Noweda	Triclosan	192709011	1
Noweda	Triclosan	192709012	1
Noweda	Triclosan	192709022	2
Noweda	Triclosan	20J30-B03-204648	1
Noweda	Triclosan	210000428009	1
Noweda	Triclosan	21000427007	1
Noweda	Triclosan	21000427008	2
Noweda	Triclosan	21000427011	2
Noweda	Triclosan	21000427017	1
Noweda	Triclosan	21000428004	1
Noweda	Triclosan	21000428009	1
Noweda	Triclosan	21000428015	1
Noweda	Triclosan	21000428020	2
Noweda	Triclosan	2101029-02	1
Noweda	Triclosan	21B25-B02-203393	1
Noweda	Triclosan	2206016-01	1
Ph.Eur 8.0	Triclosan	17081705	1
Phoenix 19.11.14	Triclosan	14121207	1
Phoenix	Triclosan	12003202	1
Phoenix	Triclosan	14205903	1
Phoenix	Triclosan	15C10-B06	1
Phoenix	Triclosan	16084614	1
Phoenix	Triclosan	1609005-02	1
Phoenix	Triclosan	16280809	2
Phoenix	Triclosan	1701032-01	1
Phoenix	Triclosan	1701032-02	1
phoenix	Triclosan	17081707	2
Phoenix	Triclosan	17081709	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Triclosan	17081721	1
Phoenix	Triclosan	17081723	2
Phoenix	Triclosan	17081726	1
Phoenix	Triclosan	17149809	1
Phoenix	Triclosan	17149820	1
Phoenix	Triclosan	17K02-B06-343547	1
Phoenix	Triclosan	18081407	1
Phoenix	Triclosan	18081408	1
Phoenix	Triclosan	18081414	1
Phoenix	Triclosan	18253705	1
Phoenix	Triclosan	18253706	1
Phoenix	Triclosan	18253708	1
Phoenix	Triclosan	18253716	2
Phoenix	Triclosan	18253717	1
Phoenix	Triclosan	18253718	1
Phoenix	Triclosan	18253721	3
Phoenix	Triclosan	1901006-01	1
Phoenix	Triclosan	1912002-02	1
Phoenix	Triclosan	21000427003	1
Phoenix	Triclosan	21000427005	1
Phoenix	Triclosan	21000427014	2
Phoenix	Triclosan	21000428011	2
Phoenix	Triclosan	21000428022	1
Phoenix	Triclosan	3417	1
Phöix	Triclosan	21000428022	2
Phönix 27.6.2019	Triclosan	18253705	1
Phönix 5.4.19	Triclosan	18253706	2
Phönix Berlin / Lamotte	Triclosan	17081711	1
Phönix Gotha	Triclosan	13391807	1
Phönix Gotha	Triclosan	1408024-01	2
Phönix Mvda 3.7.2019	Triclosan	18253714	1
Phönix/Caesar&Lorenz…	Triclosan	21000428008	2
Phönix/Caesar&Lorenz…	Triclosan	21000427005	1
Phönix/Eurho	Triclosan	2101029-01	1
Phönix/Fagon	Triclosan	15C10-B06-312981	1
Phönix	Triclosan		1
Phönix	Triclosan	12145908	1
Phönix	Triclosan	12359109	1
Phönix	Triclosan	12359111	1
Phönix	Triclosan	12L06-N01	1
Phönix	Triclosan	13A11-N03	1
Phönix	Triclosan	13H09-N01	1
Phonix	Triclosan	13L18-B35	1
Phönix	Triclosan	13L18-B35-289985	1
Phönix	Triclosan	13L18-B35-289995	2
Phönix	Triclosan	13L8-B35	1
Phönix	Triclosan	1516A-03402	1
Phönix	Triclosan	16280801	1
Phönix	Triclosan	16280811	2
Phönix	Triclosan	17081710	1
phönix	Triclosan	17081712	1
Phönix	Triclosan	17081725	1
Phönix	Triclosan	17149808	1
Phönix	Triclosan	17149815	1
Phönix	Triclosan	17149821	1
Phönix	Triclosan	17k02-b06-343544	1
Phönix	Triclosan	18081415	1
Phönix	Triclosan	182537001	1
Phönix	Triclosan	18253706	1
Phönix	Triclosan	18253718	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Triclosan	18253721	2
Phönix	Triclosan	1912002-01	1
Phönix	Triclosan	1912002-02	1
Phönix	Triclosan	192709004	2
Phönix	Triclosan	192709011	2
Phönix	Triclosan	192709012	1
Phönix	Triclosan	192709018	1
Phönix	Triclosan	192709020	3
phönix	Triclosan	21000427002	1
Phönix	Triclosan	21000427006	1
Phönix	Triclosan	21000427007	1
Phönix	Triclosan	21000427014	2
phönix	Triclosan	21000428010	1
Phönix	Triclosan	21000428022	2
phönix	Triclosan	2101029	1
Phönix	Triclosan	2206016-02	1
Phönix	Triclosan	3180	1
Raben-Apotheke Mildenau	Triclosan	13L18-B35-289984	2
Rondell Apotheke	Triclosan	11965460	1
Röntgen	Triclosan	17K02-B06-343546	1
Röntgen	Triclosan	1801049-01	1
Röntgen	Triclosan	1912002-03	2
Röntgen	Triclosan	2101029-01	2
Sana 06.11.14 EK 3,38	Triclosan	14121209	1
sana corp	Triclosan	12359106	1
sanacorb	Triclosan	18253711	1
Sanacorp 28.05.2019 5,55EUR	Triclosan	1901006-01	1
Sanacorp WE: 30.04.1…	Triclosan	1708025-01	1
Sanacorp WE:05.09.16…	Triclosan	1602003-01	2
Sanacorp	Triclosan		1
Sanacorp	Triclosan	10666066	1
Sanacorp	Triclosan	12359105	2
Sanacorp	Triclosan	12359106	1
Sanacorp	Triclosan	13247904	2
Sanacorp	Triclosan	13391807	2
Sanacorp	Triclosan	13D02-N02	1
Sanacorp	Triclosan	13H09-N01	1
sanacorp	Triclosan	13L18-B35-289987	1
Sanacorp	Triclosan	14052103	1
Sanacorp	Triclosan	14121211	1
Sanacorp	Triclosan	14121215	1
Sanacorp	Triclosan	1505009-01	1
Sanacorp	Triclosan	151004501	1
Sanacorp	Triclosan	17081717	1
Sanacorp	Triclosan	17081725	1
Sanacorp	Triclosan	17149806	1
Sanacorp	Triclosan	17149807	1
Sanacorp	Triclosan	17149808	1
Sanacorp	Triclosan	17149812	1
Sanacorp	Triclosan	17149814	1
Sanacorp	Triclosan	17149821	1
Sanacorp	Triclosan	18081405	2
Sanacorp	Triclosan	18081415	1
Sanacorp	Triclosan	18081416	1
Sanacorp	Triclosan	182537001	1
Sanacorp	Triclosan	182537002	1
Sanacorp	Triclosan	18253702	1
Sanacorp	Triclosan	18253707	1
Sanacorp	Triclosan	18253710	1
Sanacorp	Triclosan	18253711	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Triclosan	18253712	1
Sanacorp	Triclosan	18253714	1
sanacorp	Triclosan	18253726	1
sanacorp	Triclosan	1901006-02	1
Sanacorp	Triclosan	1912002-04	1
Sanacorp	Triclosan	192709003	1
Sanacorp	Triclosan	192709022	1
Sanacorp	Triclosan	21000427002	1
Sanacorp	Triclosan	21000427005	1
sanacorp	Triclosan	21000427016	1
Sanacorp	Triclosan	21000428005	1
Sanacorp	Triclosan	2101029-03	1
Sanacorp	Triclosan	2206016-02	1
Sanacorp	Triclosan	26/AKD1	1
Sanacorp	Triclosan	28/AKD4	1
Schulzendorfer-Apotheke	Triclosan	21000427011	1
Sonnenberg-Apotheke	Triclosan	13L18-B35-289995	1
Spangropharm	Triclosan	13D02-V02	1
triclosan	Triclosan	15C10-B06-310032	1
WE:02.04.2016 Sanaco…	Triclosan	15C10-B06-312982	3

- 229 602 spectra from 1514 *Apo-Ident* customers from a total of 48 539 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triclosan* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triclosan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	760	0	201 324
Type C	0	6457	8	229 602

The substance/substance group *Triclosan* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	99.8763 % (> 99.8299 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21509	22373	3,92	264,02
21591	22373	5,00	263,35
21615	22373	6,54	262,70
21856	21856	0,00	262,67
22227	22227	0,00	262,97
22373	22373	0,00	263,61
22987	22987	0,00	262,45
23915	22227	12,94	262,25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triptofano**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20336-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triptofano

Special notes

When selecting the *Triptofano* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triptofano	7	7	11

Second-stage model

For differentiation of the substance/substance group *Triptofano* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triptofano* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	194,96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triptofano* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triptofano*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triptofano	1506003	21866	60	20150630*
Euro OTC	Triptofano	1506003	21871	60	20150630*
Euro OTC	Triptofano	1712006	23876	40	20180105*
Euro OTC	Triptofano	1910016	24972	40	20191106*
Euro OTC	Triptofano	2004025	25259	40	20200720*
Euro OTC	Triptofano	2203027	26051	40	20220413*
Fagron	Triptofano	14B05-B32-293485	21784	60	AR-15-FG-009473-01
Fagron	Triptofano	17G19-B01-343931	23998	40	20170919

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

- 380 spectra of 8 reference samples from the substance/substance group *Triptofano*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 582 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 10 reference samples from the substance/substance group *Triptofano*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Triptofano	1806006	24144	40
Euro OTC	Triptofano	1812002	24426	40
Euro OTC	Triptofano	1906018	24795	40
Euro OTC	Triptofano	2009041	25421	40
Euro OTC	Triptofano	2302015	26638	40
Euro OTC	Triptofano	2401010	27148	30
Fagron	Triptofano	16E11-B03-322919	23195	40
Euro OTC	Triptofano	2203027	26051SI†	10
Euro OTC	Triptofano	2302015	26638SI	20
Euro OTC	Triptofano	2401010	27148SI	20

- 201 764 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 5 *Apo-Ident* customers from 11 batches from the substance/substance group *Triptofano*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Supplier	Substance	Batch	Spectra
Caelo	Triptofano	131046	1
Euro OTC	Triptofano	1307004-01	2
Euro OTC	Triptofano	150600302	1
Euro OTC	Triptofano	1506003-03	2
Euro OTC	Triptofano	1712006-01	1
Euro OTC	Triptofano	180600601	1
Euro OTC	Triptofano	190601801	1
Euro OTC	Triptofano	2000402501	1
Euro OTC	Triptofano	2004025-01	1
Euro OTC	Triptofano	2203027-01	1
euroct/gehe	Triptofano	1212010-01	5

- 236 050 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triptofano* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triptofano* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	320	0	201 764
Type C	0	17	0	236 050

The substance/substance group *Triptofano* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21784	21784	0,00	333,97
21866	21866	0,00	333,90
21871	21871	0,00	332,70
23876	23876	0,00	334,32
23998	24972	4,62	336,17
24972	24972	0,00	334,42
25259	25259	0,00	331,01
26051	26051	0,00	328,86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Trometamol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20004-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Trometamol; Trometamina; Trometamolum

Special notes

When selecting the *Trometamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Trometamol	9	8	227

Second-stage model

For differentiation of the substance/substance group *Trometamol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Trometamol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Arginina	120,42	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Trometamol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Trometamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Trometamol	14050002	21358	40	20140220
Caelo	Trometamol	161688	22629	40	20160615*
Caelo	Trometamol	16168810	23498	40	20160615
Caelo	Trometamol	22000894	26112	40	20220331*
Caelo	Trometamol	22000894	26112SI	20	20220331*
Caelo	Trometamol	22002697	26360	40	20220921*
Caelo	Trometamol	22002697	26360SI	20	20220921*
Caelo	Trometamol	23002408	26972	40	20231012*
Euro OTC	Trometamol	1803016	24063	40	20180320*
Fagron	Trometamol	13E22-N05	20856	40	AR-17-FG-016395-01
Fagron	Trometamol	18A23-B10-351258	24816	40	20180306

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 11 reference samples from the substance/substance group *Trometamol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 10 reference samples from the substance/substance group *Trometamol*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Trometamol	173208	23787	40
Caelo	Trometamol	190887	25206	40
Caelo	Trometamol	20002276	25640	40
Caelo	Trometamol	23000494	26709	40
Caelo	Trometamol	24000307	27260	40
Euro OTC	Trometamol	2303016	26650	40
Fagron	Trometamol	17A16-B04-334121	23516	40
Fagron	Trometamol	22I20-B05-225357	26465	40
Fagron	Trometamol	17A16-B04-334121	23517	40
Fagron	Trometamol	22I20-B05-225357	26465SI	20

- 201 704 spectra from a total of 4037 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1513 spectra from 758 *Apo-Ident* customers from 235 batches from the substance/substance group *Trometamol*.

- Among them are spectra of independent samples from 225 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Trometamol		1
	Trometamol	2100283014	1
	Trometamol	21002838011	3
	Trometamol	21002838014	4
	Trometamol	22000894006	1
	Trometamol	22002697006	6
	Trometamol	22002697016	9
	Trometamol	23000494005	12
	Trometamol	23000494007	2
	Trometamol	23001254008	3
	Trometamol	23003309002	5
AHC	Trometamol	2300154008	1
AHD	Trometamol	13095910	1
AHD	Trometamol	17320801	1
AHD	Trometamol	18197103	1
Alliance	Trometamol	21002838005	1
Anzag	Trometamol	12113512	1
ANZAG	Trometamol	12113512	1
Anzag	Trometamol	13095911	1
Bartschat	Trometamol	190887007	1
Bombastus	Trometamol	17320811	1
Bombastus	Trometamol	18197103	1
Caelo	Trometamol		6
Caelo	Trometamol	1001312519	1
Caelo	Trometamol	1018U-02519	1
Caelo	Trometamol	11160706	1
Caelo	Trometamol	11160707	1
Caelo	Trometamol	11160711	1
Caelo	Trometamol	11160714	2
Caelo	Trometamol	1119I-02519	1
Caelo	Trometamol	11376005	5
Caelo	Trometamol	11376006	8
Caelo	Trometamol	1180116	1
Caelo	Trometamol	12113502	2
Caelo	Trometamol	12113506	9
Caelo	Trometamol	12113507	3
Caelo	Trometamol	12113510	2
Caelo	Trometamol	12113511	1
Caelo	Trometamol	12113512	10
Caelo	Trometamol	12113515	4
Caelo	Trometamol	13051401	1
Caelo	Trometamol	13095901	10
Caelo	Trometamol	13095902	11
Caelo	Trometamol	13095905	1
Caelo	Trometamol	13095910	5
Caelo	Trometamol	13095911	12
Caelo	Trometamol	13095912	14
Caelo	Trometamol	13095913	3
Caelo	Trometamol	13095915	4
Caelo	Trometamol	13339103	9
Caelo	Trometamol	13339107	8
Caelo	Trometamol	13339108	11
Caelo	Trometamol	1339103	1
Caelo	Trometamol	13C-08-N07	1
Caelo	Trometamol	14050002	7
Caelo	Trometamol	14050003	2
Caelo	Trometamol	14050004	4
Caelo	Trometamol	14050006	1
Caelo	Trometamol	14332402	23
Caelo	Trometamol	14332403	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Trometamol	14332404	1
Caelo	Trometamol	14F19B03304293	1
Caelo	Trometamol	14F19-B03-304293	1
Caelo	Trometamol	150703	1
Caelo	Trometamol	15070304	10
Caelo	Trometamol	15070307	4
Caelo	Trometamol	15070308	29
Caelo	Trometamol	15070309	1
Caelo	Trometamol	15070311	27
Caelo	Trometamol	15094401	15
Caelo	Trometamol	15094404	1
Caelo	Trometamol	15277602	1
Caelo	Trometamol	15377602	25
Caelo	Trometamol	15377604	2
Caelo	Trometamol	15377605	1
Caelo	Trometamol	15377607	31
Caelo	Trometamol	15377611	31
Caelo	Trometamol	15377661	1
Caelo	Trometamol	161013T/15377607	1
Caelo	Trometamol	161668810	1
Caelo	Trometamol	16168801	1
Caelo	Trometamol	16168807	1
Caelo	Trometamol	16168810	40
Caelo	Trometamol	16168810-11417/3	1
Caelo	Trometamol	16168810-6417/1	1
Caelo	Trometamol	16168812	2
Caelo	Trometamol	16168816	2
Caelo	Trometamol	16168819	18
Caelo	Trometamol	16168820	27
Caelo	Trometamol	16168825	2
Caelo	Trometamol	1618810	2
Caelo	Trometamol	16D14-b-09-328729	1
Caelo	Trometamol	17020304	16
Caelo	Trometamol	17053184	1
Caelo	Trometamol	171978	1
Caelo	Trometamol	17197804	30
Caelo	Trometamol	17197806	3
Caelo	Trometamol	17197809	9
Caelo	Trometamol	1719804	1
Caelo	Trometamol	1730804	1
Caelo	Trometamol	173200816	1
Caelo	Trometamol	17320611	1
Caelo	Trometamol	17320801	41
Caelo	Trometamol	17320801/1160518	1
Caelo	Trometamol	17320802	2
Caelo	Trometamol	17320804	44
Caelo	Trometamol	17320810	2
Caelo	Trometamol	17320811	56
Caelo	Trometamol	17320816	33
Caelo	Trometamol	1732816	1
Caelo	Trometamol	17A16-B14	1
Caelo	Trometamol	18041815	1
Caelo	Trometamol	18081503	1
Caelo	Trometamol	181016182	1
Caelo	Trometamol	18197101	14
Caelo	Trometamol	18197103	23
Caelo	Trometamol	18197109	26
Caelo	Trometamol	18197414	1
Caelo	Trometamol	1897103	1
Caelo	Trometamol	18A23-B10-347884	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Trometamol	18A23-B10-349673	1
Caelo	Trometamol	18H13-B04	1
Caelo	Trometamol	190502205	1
Caelo	Trometamol	190887006	2
Caelo	Trometamol	190887007	38
Caelo	Trometamol	190887009	1
Caelo	Trometamol	19088702	3
Caelo	Trometamol	19088705	40
Caelo	Trometamol	19088706	1
Caelo	Trometamol	19197103	1
Caelo	Trometamol	200002276005	1
Caelo	Trometamol	200004247003	1
Caelo	Trometamol	20002276003	1
Caelo	Trometamol	20002276004	1
Caelo	Trometamol	20002276005	34
Caelo	Trometamol	20002276006	28
Caelo	Trometamol	20002276009	1
Caelo	Trometamol	2000424016	1
Caelo	Trometamol	20004247002	1
Caelo	Trometamol	20004247003	18
Caelo	Trometamol	20004247004	1
Caelo	Trometamol	20004247010	3
Caelo	Trometamol	20004247012	1
Caelo	Trometamol	20004247016	17
Caelo	Trometamol	2002276005	1
Caelo	Trometamol	2002276006	1
Caelo	Trometamol	2004247016	1
Caelo	Trometamol	21000487001	50
Caelo	Trometamol	2100048701	1
Caelo	Trometamol	21002838005	15
Caelo	Trometamol	21002838009	1
Caelo	Trometamol	21002838011	9
Caelo	Trometamol	21002838013	1
Caelo	Trometamol	21002838014	2
Caelo	Trometamol	21082013A	1
Caelo	Trometamol	213E-02519	1
Caelo	Trometamol	215I-02519	1
Caelo	Trometamol	22002697006	2
Caelo	Trometamol	22002697016	1
Caelo	Trometamol	23062015B	1
Caelo	Trometamol	26111201	1
Caelo	Trometamol	27111304	1
Caelo	Trometamol	314Q2519	1
Caelo	Trometamol	318A-02519	1
Caelo	Trometamol	3308	1
Caelo	Trometamol	3439	1
Caelo	Trometamol	3713E-02519	1
Caelo	Trometamol	4616M-02519	1
Caelo	Trometamol	5012M-02519	1
Caelo	Trometamol	5315I-02519	1
Caelo	Trometamol	8031301	1
Caelo	Trometamol	8721	1
Caelo	Trometamol	914I-02519	1
Caeolo/Sanacorp	Trometamol	18197101	1
Caesar & Loretz / Sa…	Trometamol	20002276005	1
Caesar & Loretz GmbH…	Trometamol	21002838005	1
Caesar & Loretz GmbH…	Trometamol	21002838005	1
Caesar & Loretz GmbH…	Trometamol	18197101	1
Caesar & Loretz GmbH…	Trometamol	19088705	1
Caesar & Loretz GmbH…	Trometamol	21002838011	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Trometamol	19088705	1
Caesar & Loretz GmbH...	Trometamol	21000487001	2
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	22002697016	1
Caesar & Loretz GmbH...	Trometamol	19088705	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	E300003986	1
Caesar & Loretz GmbH...	Trometamol	11160714	1
Caesar & Loretz GmbH...	Trometamol	13095902	1
Caesar & Loretz GmbH/ AHD	Trometamol	18197108	1
Caesar & Loretz GmbH...	Trometamol	20002276005	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	190887007	1
Caesar & Loretz GmbH...	Trometamol	20002276005	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH/Gehe	Trometamol	190887007	1
Caesar & Loretz GmbH/Gehe	Trometamol	19088705	2
Caesar & Loretz GmbH/Gehe	Trometamol	20002276006	1
Caesar & Loretz GmbH/Gehe	Trometamol	20004247016	1
Caesar & Loretz GmbH...	Trometamol	21000487001	2
Caesar & Loretz GmbH/Kehr	Trometamol	18197103	1
Caesar & Loretz GmbH/L50	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	19088705	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	21002838011	1
Caesar & Loretz GmbH/Phoe	Trometamol	190887006	1
Caesar & Loretz GmbH...	Trometamol	190887007	1
Caesar & Loretz GmbH...	Trometamol	20002276006	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	17320816	1
Caesar & Loretz GmbH...	Trometamol	190887	1
Caesar & Loretz GmbH...	Trometamol	20004247003	2
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH...	Trometamol	22002697006	1
Caesar & Loretz GmbH...	Trometamol	18197103	1
Caesar & Loretz GmbH...	Trometamol	18197103	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH	Trometamol	14050003	1
Caesar & Loretz GmbH	Trometamol	17320811	1
Caesar & Loretz GmbH	Trometamol	18197101	2
Caesar & Loretz GmbH	Trometamol	18197103	3
Caesar & Loretz GmbH	Trometamol	18197109	6
Caesar & Loretz GmbH	Trometamol	190887006	3
Caesar & Loretz GmbH	Trometamol	190887007	17
Caesar & Loretz GmbH	Trometamol	19088702	1
Caesar & Loretz GmbH	Trometamol	19088705	11
Caesar & Loretz GmbH	Trometamol	20002276005	10
Caesar & Loretz GmbH	Trometamol	20002276006	4
Caesar & Loretz GmbH	Trometamol	20004247003	7
Caesar & Loretz GmbH	Trometamol	20004247010	2
Caesar & Loretz GmbH	Trometamol	20004247016	5
Caesar & Loretz GmbH	Trometamol	20005576005	1
Caesar & Loretz GmbH	Trometamol	21000487001	20
Caesar & Loretz GmbH	Trometamol	21002838005	9
Caesar & Loretz GmbH	Trometamol	21002838011	5
Caesar & Loretz/Geil...	Trometamol	20004247003	1
Caesar & Loretz/Phoenix	Trometamol	21000487001	1
Caesar & Loretz	Trometamol	16168819	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar / Gehe	Trometamol	15377607	1
Caesar Loretz	Trometamol	190887007	1
Caesar&Loretz	Trometamol	16168820	1
Calo, Hilden/ Phönix	Trometamol	18197109	1
Cealo/Anzag	Trometamol	18197103	1
Cealo	Trometamol	2002276005	1
Celo/Phönix	Trometamol	16168810	1
E300025088	Trometamol	21B15-F03-377086	2
Euro OTC	Trometamol	1203005-02	3
Euro OTC	Trometamol	15070308	1
Euro OTC	Trometamol	15377602	1
Euro OTC	Trometamol	16168810	1
Euro OTC	Trometamol	17197809	2
Euro OTC	Trometamol	17320804	1
Euro OTC	Trometamol	17320816	1
Euro OTC	Trometamol	18197101	1
Fagron	Trometamol	10B26-N05	1
Fagron	Trometamol	12E25-B40	1
Fagron	Trometamol	12I27-N03	1
Fagron	Trometamol	12I27-No3	1
Fagron	Trometamol	12K14-N05	2
Fagron	Trometamol	12k14no5	1
Fagron	Trometamol	13/19-B02	1
Fagron	Trometamol	13/19-B02-286158	3
Fagron	Trometamol	13/19-B02-293595	3
Fagron	Trometamol	13119-B02	1
Fagron	Trometamol	13C08-N07	3
Fagron	Trometamol	13E22-N05	5
Fagron	Trometamol	13I19-B02	1
Fagron	Trometamol	13I19-B02-286158	1
Fagron	Trometamol	13I19-B02-293595	2
Fagron	Trometamol	13l19-B02-286158	1
Fagron	Trometamol	14F19-B03	1
Fagron	Trometamol	14F19-B03-304293	4
Fagron	Trometamol	16(18A23-B10-347884	1
Fagron	Trometamol	16D14-B09	1
Fagron	Trometamol	16d14-b09-328729	1
Fagron	Trometamol	16D14-B09-328729	2
Fagron	Trometamol	17320816	1
Fagron	Trometamol	17A16-B04	2
Fagron	Trometamol	17A16-B04-334121	4
Fagron	Trometamol	17A16-B04-337589	1
Fagron	Trometamol	17A16-B04-340796	4
Fagron	Trometamol	17A16-B04-345550	1
Fagron	Trometamol	18A23-B10-347884	3
Fagron	Trometamol	18A23-B10-349673	5
Fagron	Trometamol	18A23-B10-351258	5
Fagron	Trometamol	18A-23-B10-351258	1
Fagron	Trometamol	18H13-B04-363961	3
Fagron	Trometamol	18H13-B04-363962	1
Fagron	Trometamol	18H13-B04-370289	4
Fagron	Trometamol	20H05-F06-373066	2
Fagron	Trometamol	20H05-F06-373351	2
Fagron	Trometamol	21E18-B03-215278	6
Fagron	Trometamol	21I30-B05	1
Fagron	Trometamol	220728(E300025088)	1
Fagron	Trometamol	294101	1
Fagron	Trometamol	3377086	1
Fagron	Trometamol	610I-02519	1
Fagron	Trometamol	8386E050	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Trometamol	8386H037	1
Fagron	Trometamol	8386J009	2
Fagron	Trometamol	8386K059	1
Fagron	Trometamol	E300003986	2
Fagron	Trometamol	E300021548	3
Fagron	Trometamol	E30021548	1
Fagron	Trometamol	F06-3730607	1
Fagron	Trometamol	TM284375698	1
fargon/gehe	Trometamol	17K23-B04-355709	1
Fargon/Kehr	Trometamol	17A16-B04-337589	1
Fiebig	Trometamol	16168825	1
Fiebig	Trometamol	17320804	1
Gatt-Koller	Trometamol	1801776	1
Gatt-Koller	Trometamol	1804167	1
Gehe 04.11.21 EK:6,97EUR	Trometamol	211105TR	1
Gehe/Fragron	Trometamol	18A23-B10	1
Gehe	Trometamol	11025103	1
Gehe	Trometamol	11160708	1
Gehe	Trometamol	13E22-N05	1
Gehe	Trometamol	15070311	1
Gehe	Trometamol	15377611	1
GEHE	Trometamol	16168810	1
Gehe	Trometamol	17020304	1
Gehe	Trometamol	17A16-B04-345550	1
Gehe	Trometamol	1819701	1
Gehe	Trometamol	18197101	1
GEHE	Trometamol	18A23-B10	1
Gehe	Trometamol	190887007	1
Gehe	Trometamol	19088705	1
Gehe	Trometamol	21000487001	1
Gehe	Trometamol	21002838005	1
Gehe	Trometamol	22002697016	1
Jenne	Trometamol	17320811	1
Klenk	Trometamol	13095902	2
Krieger am 17.08.2018	Trometamol	17320801	1
Merck	Trometamol	8386F017	1
Merck	Trometamol	E300000206913	2
Midas	Trometamol	17197804	1
Nachprüfung	Trometamol	3082019-2	1
Noweda	Trometamol	11376005	1
Noweda	Trometamol	18197101	1
Noweda	Trometamol	19088705	1
Noweda	Trometamol	21002838011	1
Noweda	Trometamol	22002697006	1
Noweda	Trometamol	23001254010	1
Phoenix Hannover	Trometamol	20002276006	1
Phoenix/Cealo	Trometamol	16168825	1
Phoenix	Trometamol	16168819	1
Phoenix	Trometamol	17197804	1
Phoenix	Trometamol	17320804	1
Phoenix	Trometamol	18197109	1
Phoenix	Trometamol	23000494005	1
Phoenix	Trometamol	3039	1
Phoenix	Trometamol	3114	1
Phoenix	Trometamol	3218	1
Phoenix	Trometamol	3409	1
Phönix Gotha	Trometamol	13/19-B02-286158	1
Phönix Gotha	Trometamol	1319-B02-286158	1
Phönix	Trometamol	12113512	1
Phönix	Trometamol	13095912	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Trometamol	14332402	1
Phönix	Trometamol	16168819	1
phönix	Trometamol	17197804	1
Phönix	Trometamol	17197804	1
Phönix	Trometamol	17320804	2
Phönix	Trometamol	17320816	1
Phönix	Trometamol	20002276005	1
PHÖNIX	Trometamol	20004247003	1
phönix	Trometamol	21002838005	1
Phönix	Trometamol	23000494005	1
Post Apotheke	Trometamol	18197101	1
Röntgen	Trometamol	17320801	1
Sanacorp	Trometamol	12113506	1
Sanacorp	Trometamol	13095912	1
Sanacorp	Trometamol	15377602	1
Sanacorp	Trometamol	16168820	1
Sanacorp	Trometamol	17197809	1
Sanacorp	Trometamol	17320804	1
Sanacorp	Trometamol	18197103	1
Sanacorp	Trometamol	21000487001	3
Sanacorp	Trometamol	22002697006	2
Sanacorp	Trometamol	22002697010	1
Sanacorp	Trometamol	23000494005	1
Sanacorp	Trometamol	3686G018	1
Sanacorp	Trometamol	8386H037	1
Sanocorp WE:21.05.16…	Trometamol	15070311	2
Spangro 25.02.2019	Trometamol	18197101	1
vwr chemicals	Trometamol	E300027934	1

- 234 554 spectra from 1515 *Apo-Ident* customers from a total of 49 026 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Trometamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Trometamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	380	0	201 704
Type C	0	1513	0	234 554

The substance/substance group *Trometamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.6034 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20856	20856	0,00	231,05
21358	26112	6,01	212,54
22629	22629	0,00	217,28
23498	22629	10,88	237,86
24063	24063	0,00	225,42
24816	22629	9,67	223,29
26112	26112	0,00	214,44
26360	26360	0,00	207,18
26972	26972	0,00	242,64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tropicalamida**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20598-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tropicalamida; Tropicamidum

Special notes

When selecting the *Tropicalamida* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tropicalamida	6	7	49

Second-stage model

For differentiation of the substance/substance group *Tropicalamida* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tropicalamida* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	130,67	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tropicalamida* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tropicalamida*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tropicalamida	2001016	25299	40	20200807*
Euro OTC	Tropicalamida	2106001	25709	50	20210720*
Fagron	Tropicalamida	14D23-B04-293294	21685	60	AR-15-FG-001641-01
Fagron	Tropicalamida	16G19-B05-324829	22885	40	20160905
Fagron	Tropicalamida	17J06-B04-341322	23982	40	1807428
Fagron	Tropicalamida	21A11-F03-376917	25665	50	20210120

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Tropicalamida*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 11 reference samples from the substance/substance group *Tropicalamida*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Tropicalamida	APFP/TD003/09/17/TR	23983	40
Euro OTC	Tropicalamida	2203001	26043	40
Euro OTC	Tropicalamida	2204015	26223	40
Euro OTC	Tropicalamida	2402034	27209	40
Euro OTC	Tropicalamida	2309014	27213	40
Fagron	Tropicalamida	17D25-B07-336833	23506	40
Fagron	Tropicalamida	18H14-B06-362792	25367	40
Euro OTC	Tropicalamida	2106001	25709SI†	10
Euro OTC	Tropicalamida	2203001	26043SI	40
Euro OTC	Tropicalamida	2204015	26223SI	40
Fagron	Tropicalamida	21A11-F03-376917	25665SI†	10

- 201 704 spectra from a total of 4036 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 119 spectra from 30 *Apo-Ident* customers from 51 batches from the substance/substance group *Tropicalamida*.
- Among them are spectra of independent samples from 49 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Tropicalamida	22D14-B02-220415	1
	Tropicalamida	22L08-B03-222105	1
ALH	Tropicalamida	15F18-B04-310971	1
Caelo	Tropicalamida	17J06-B04-348766	1
Euro OTC	Tropicalamida	2001016-01	1
Euro OTC	Tropicalamida	2106001-01	2
Fagron	Tropicalamida	1/06/2000	1
Fagron	Tropicalamida	12F18-N06	4
Fagron	Tropicalamida	12l04-n03	1
Fagron	Tropicalamida	14D23B04293294	1
Fagron	Tropicalamida	14l04-b02-315694	1
Fagron	Tropicalamida	14L04B02315694	1
Fagron	Tropicalamida	14L04-B02-315694	2
Fagron	Tropicalamida	15F18-B04	1
Fagron	Tropicalamida	15F18-B04-308977	1
Fagron	Tropicalamida	15F18B04312001	1
Fagron	Tropicalamida	15F18-B04-312001	1
Fagron	Tropicalamida	17D25-B07-336833	6
Fagron	Tropicalamida	17J06-B04	2
Fagron	Tropicalamida	17J06-B04-341323	5
Fagron	Tropicalamida	17J06-B04-343279	2
Fagron	Tropicalamida	17J06-B04-348766	4
Fagron	Tropicalamida	17J06-B04-352344	2
Fagron	Tropicalamida	17J06-B04-354804	3
Fagron	Tropicalamida	18H014-B06-357220	1
Fagron	Tropicalamida	18H14-B06	1
Fagron	Tropicalamida	18H14-B06-357220	5
Fagron	Tropicalamida	18H14-B06-359927	6
Fagron	Tropicalamida	18H14-B06-362475	3
Fagron	Tropicalamida	18H14-B06-362476	8
Fagron	Tropicalamida	18H14-B06-362792	1
Fagron	Tropicalamida	18H14-B06-362794	7
Fagron	Tropicalamida	18H14-B06-362796	1
Fagron	Tropicalamida	18H14-B06-363716	1
Fagron	Tropicalamida	18H14-B06-369986	1
Fagron	Tropicalamida	2/05/1008	1
Fagron	Tropicalamida	20021302	1
Fagron	Tropicalamida	20C06F03-3699807	1
Fagron	Tropicalamida	20C06-F03-369987	3
Fagron	Tropicalamida	20C06-F03-371990	2
Fagron	Tropicalamida	21H13-B17-213648	2
Fagron	Tropicalamida	21H13-B17-216490	6
Fagron	Tropicalamida	21J15-B04-216491	2
Fagron	Tropicalamida	23071508	1
Fagron	Tropicalamida	B06-3627902	2
Fagron	Tropicalamida	B06-3627904	1
Fagron	Tropicalamida	B06-362794	1
Fagron	Tropicalamida	F03-3699807	2
Fagron	Tropicalamida	FP/TD/003/09/17	1
Gehe	Tropicalamida	15F18-B04	1
Gehe	Tropicalamida	15F-18B-04	1
GEHE	Tropicalamida	18H14-B06	2
Phoenix	Tropicalamida	14L04-B02	2
PHÖNIX	Tropicalamida	16G19-B05-324829	1
PHÖNIX	Tropicalamida	17J06-B04	5

- 235 948 spectra from 1515 *Apo-Ident* customers from a total of 49 207 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tropicalamida* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tropicalamida* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	380	0	201 704
Type C	0	118	1	235 948

The substance/substance group *Tropicalamida* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	99.1597 % (> 96.6387 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21685	21685	0,00	221,96
22885	23982	11,19	220,34
23982	23982	0,00	223,29
25299	25299	0,00	221,12
25665	25709	5,24	219,17
25709	25709	0,00	220,19

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ubidecarenona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20392-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ubidecarenona; Coenzima Q10

Special notes

When selecting the *Ubidecarenona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ubidecarenona	11	16	31

Second-stage model

For differentiation of the substance/substance group *Ubidecarenona* the following second-stage model is used:

- Submodelo 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ubidecarenona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbômero	117,19	–
⋮	⋮	⋮
Progesterona	>50	101,30
Ácido fusídico	>50	110,40
Espironolactona	>50	117,42
Iodopovidona	>50	134,28
Propionato de testosterona	>50	140,33
Povidona	>50	199,47

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ubidecarenona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ubidecarenona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ubidecarenona	14004504	21388	60	AR-15-FG-009220-01
Caelo	Ubidecarenona	17209402	23580	40	20170823
Caelo	Ubidecarenona	17209402	23581	40	20170823
Caelo	Ubidecarenona	172094	23647	35	20170823*
Euro OTC	Ubidecarenona	1205029-01	21247	40	20121009
Euro OTC	Ubidecarenona	1605030	22696	40	20160623*
Euro OTC	Ubidecarenona	1703026	23127	40	20170406*
Euro OTC	Ubidecarenona	1801019	23881	40	20180126*
Euro OTC	Ubidecarenona	2004036	25282	40	20200618*
Euro OTC	Ubidecarenona	2010017	25544	40	20210108*
Fagron	Ubidecarenona	16G26-B01-331742	23161	40	20170110
Fagron	Ubidecarenona	18J24-B01-357225	24688	40	20181121

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 495 spectra of 12 reference samples from the substance/substance group *Ubidecarenona*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 467 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 720 spectra of 21 reference samples from the substance/substance group *Ubidecarenona*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ubidecarenona	182298	24281	40
Caelo	Ubidecarenona	21002685002	25975	40
Caelo	Ubidecarenona	22002474	26351	40
Euro OTC	Ubidecarenona	1802025	24074	40
Euro OTC	Ubidecarenona	1804020	24116	40
Euro OTC	Ubidecarenona	1810012	24305	40
Euro OTC	Ubidecarenona	1902030	24630	40
Euro OTC	Ubidecarenona	2003002	25142	40
Euro OTC	Ubidecarenona	2101025	25541	40
Euro OTC	Ubidecarenona	2110011	25894	50
Euro OTC	Ubidecarenona	2205006	26191	40
Euro OTC	Ubidecarenona	2303015	26642	40
Euro OTC	Ubidecarenona	2402030	27215	40
Euro OTC	Ubidecarenona	2410012	27460	40
Fagron	Ubidecarenona	21K09-B08-215716	26075	40
Fagron	Ubidecarenona	23H07-B02-223783	27035	40
Caelo	Ubidecarenona	21002685002	25975SI	10
Caelo	Ubidecarenona	22002474	26351SI	20
Euro OTC	Ubidecarenona	2110011	25894SI	10
Euro OTC	Ubidecarenona	2205006	26191SI	20
Fagron	Ubidecarenona	21K09-B08-215716	26075SI	10

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 364 spectra from a total of 4029 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 46 spectra from 18 *Apo-Ident* customers from 32 batches from the substance/substance group *Ubidecarenona*.

- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ubidecarenona	2101025-03	1
Audor Pharma	Ubidecarenona	APSCFQ150614C	1
Audor Pharma	Ubidecarenona	APSZFQ150614C	1
Audor Pharma	Ubidecarenona	APSZFQ170617C	1
Caelo	Ubidecarenona	18048401	1
Caesar & Loretz GmbH	Ubidecarenona	20003319001	1
Dr. Behr	Ubidecarenona	WE18020018	1
Euro OTC	Ubidecarenona	1014E-07029	1
Euro OTC	Ubidecarenona	1403020-02	1
Euro OTC	Ubidecarenona	1515M-07029	1
Euro OTC	Ubidecarenona	1605030-01	3
Euro OTC	Ubidecarenona	1801019-01	1
Euro OTC	Ubidecarenona	1802025-01	4
Euro OTC	Ubidecarenona	1804020-01	1
Euro OTC	Ubidecarenona	1810012-01	2
Euro OTC	Ubidecarenona	1902030-01	3
Euro OTC	Ubidecarenona	1902030-02	3
Euro OTC	Ubidecarenona	2110011-01	1
Euro OTC	Ubidecarenona	L1403020-01	1
Fagron	Ubidecarenona	14E12-B06-293861	1
Fagron	Ubidecarenona	14H26-B04-298244	1
Fagron	Ubidecarenona	16B10-B05-327606	1
Fagron	Ubidecarenona	16G26-B01	3
Fagron	Ubidecarenona	16G26-B01-344334	2
Fagron	Ubidecarenona	18A16-B03	2
Fagron	Ubidecarenona	18a16-b03-351350	1
Fagron	Ubidecarenona	18A16-B03-351350	1
Fagron	Ubidecarenona	18J24-B01	1
Fragon	Ubidecarenona	18J24-B01-362124	1
Sanacorp	Ubidecarenona	2004036-02	1
Sanacorp	Ubidecarenona	2101025-01	1
Sanacorp	Ubidecarenona	51-1911123	1

- 236 021 spectra from 1515 *Apo-Ident* customers from a total of 49 227 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ubidecarenona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ubidecarenona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	495	0	152 467
Type B	0	720	0	201 364
Type C	0	43	3	236 021

The substance/substance group *Ubidecarenona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7879 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1667 %)
Type C	100.0000 % (> 99.9007 %)	93.4783 % (> 86.9565 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21247	21388	6,24	134,58
21388	21388	0,00	135,07
22696	22696	0,00	138,77
23127	23127	0,00	136,36
23161	23127	2,25	135,08
23580	22696	4,74	132,30
23581	21388	4,98	132,73
23647	23647	0,00	135,54
23881	23881	0,00	137,67
24688	23881	5,65	135,67
25282	25282	0,00	137,59
25544	25544	0,00	137,52

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ureia**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20017-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ureia; Ureum

Special notes

When selecting the *Ureia* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ureia	11	18	599

Second-stage model

For differentiation of the substance/substance group *Ureia* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ureia* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	119,93	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ureia* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ureia*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ureia	15154103	22315	60	20150722
Caelo	Ureia	15154103	22315SI	60	20150722
Caelo	Ureia	161074	22466	60	20160509*
Caelo	Ureia	170216	23033	40	20170202*
Caelo	Ureia	18023003	24294	40	20180216
Euro OTC	Ureia	1404024-01	21537	60	20140519
Euro OTC	Ureia	1601044	22376	40	20160208*
Euro OTC	Ureia	1604044	22552	40	20160512*
Euro OTC	Ureia	2102002	25549	40	20210205*
Euro OTC	Ureia	2301020	26518	40	20230125*
Euro OTC	Ureia	2301020	26518SI	40	20230125*
Fagron	Ureia	12F25-N05	20712	40	20120724
Fagron	Ureia	14I18-B03-303581	22317	60	20141003
Fagron	Ureia	14I18-B03-303581	22317SI	60	20141003

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Type A All calibration spectra.

- 680 spectra of 14 reference samples from the substance/substance group *Ureia*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 282 spectra from a total of 2831 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1340 spectra of 33 reference samples from the substance/substance group *Ureia*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ureia	180242	24042	40
Caelo	Ureia	180230	24043	40
Caelo	Ureia	190316	24550	40
Caelo	Ureia	21002313009	25930	40
Caelo	Ureia	22002605	26355	40
Caelo	Ureia	23001146	26892	40
Caelo	Ureia	24001776	27330	40
Euro OTC	Ureia	1702023	23156	40
Euro OTC	Ureia	1707015	23535	40
Euro OTC	Ureia	1804007	24078	40
Euro OTC	Ureia	1811012	24340	40
Euro OTC	Ureia	1908016	24865	40
Euro OTC	Ureia	2004010	25143	40
Euro OTC	Ureia	2109001	25829	50
Euro OTC	Ureia	2205037	26198	40
Euro OTC	Ureia	2309011	26923	40
Fagron	Ureia	21L08-B04-219541	26165	40
Fagron	Ureia	23C21-B01-228852	27173	40
Caelo	Ureia	170216	23033SI†	40
Caelo	Ureia	18023003	24294SI†	40
Caelo	Ureia	21002313009	25930SI	40
Caelo	Ureia	22002605	26355SI	40
Caelo	Ureia	23001146	26892SI	40
Caelo	Ureia	24001776	27330SI	40
Euro OTC	Ureia	1604044	22552SI†	40
Euro OTC	Ureia	1702023	23156SI	40
Euro OTC	Ureia	1804007	24078SI	40
Euro OTC	Ureia	1811012	24340SI	40
Euro OTC	Ureia	2109001	25829SI	50

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ureia	2205037	26198SI	40
Euro OTC	Ureia	2309011	26923SI	40
Fagron	Ureia	21L08-B04-219541	26165SI	40
Fagron	Ureia	23C21-B01-228852	27173SI	40

- 200 744 spectra from a total of 4024 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6622 spectra from 1345 *Apo-Ident* customers from 617 batches from the substance/substance group *Ureia*.
- Among them are spectra of independent samples from 596 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ureia		3
	Ureia	12111808	1
	Ureia	20003817006	1
	Ureia	210002313015	1
	Ureia	21002313006	1
	Ureia	21002313009	1
	Ureia	21002313015	1
	Ureia	21002313017	1
	Ureia	2109001-01	1
	Ureia	21L08-B04-219541	1
	Ureia	22002605001	10
	Ureia	22002605003	13
	Ureia	22002605005	8
	Ureia	22002605008	2
	Ureia	22002605009	20
	Ureia	22002605010	23
	Ureia	22002605011	1
	Ureia	2200265001	1
	Ureia	2200605009	1
	Ureia	2205037-01	3
	Ureia	2205037-02	2
	Ureia	22L02-B12-226179	2
	Ureia	23001146001	22
	Ureia	23001146002	20
	Ureia	23001146003	4
	Ureia	23003219004	2
	Ureia	23003219005	3
	Ureia	23003219010	1
	Ureia	23003219011	4
	Ureia	23003219012	1
	Ureia	2301020-01	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Ureia	2301020-02	1
	Ureia	2309011-01	1
	Ureia	23J00550	1
	Ureia	34567	1
	Ureia	B12-2261709	1
	Ureia	V034-22022	1
10,68	Ureia	23001146003	1
ACM	Ureia	KNC0236J16	2
ACM	Ureia	KNC0557J15	3
ACM	Ureia	KNC1795J14	1
AEP	Ureia	22002605001	2
Aep	Ureia	23003219011	1
AHC	Ureia	15154110	1
AHD	Ureia	14E07-B05-293469	1
AHD	Ureia	16107428	1
AHD	Ureia	18023003	1
AHD	Ureia	18023007	2
AHD	Ureia	21002313017	1
AHD	Ureia	2109001-01	1
AHD	Ureia	22002605010	1
AHD	Ureia	2205037-01	1
AHD	Ureia	22H29-B03-223930	1
AHD	Ureia	23001146001	1
AHD	Ureia	23003219005	1
AHD	Ureia	23003219012	1
AHD	Ureia	2301020-01	2
AHD	Ureia	2309011-01	1
AHD	Ureia	3514E-02544	1
Ahde 27.11.17	Ureia	16107422	1
Alliance health	Ureia	14E07-B05-297167	1
Alliance Healthcare	Ureia	12111823	1
Alliance Healthcare	Ureia	190316003	1
Alliance Healthcare	Ureia	19031609	1
Alliance Healthcare	Ureia	20003817002	1
Alliance Healthcare	Ureia	22002605002	1
Alliance Healthcare	Ureia	22002605010	1
Alliance	Ureia	102002-012	1
Alliance	Ureia	21002313006	1
Alliance	Ureia	21002313015	1
Alliance	Ureia	23001146001	1
Allianz Healthcare	Ureia	19031604	1
Anzag / Noweda	Ureia	13064206	1
Anzag 17.04.13 ek:6,84EUR	Ureia	12111823	1
Anzag/Henry Lamotte	Ureia	13-18-B03-303581	1
Anzag	Ureia	12111801	1
anzag	Ureia	14E07-B05-293469	1
Anzag	Ureia	16107411	1
Anzag	Ureia	19031614	1
Anzag	Ureia	22002605009	1
Anzag	Ureia	22002605010	1
Apotheke	Ureia	920A-07062	1
Audor Pharma	Ureia	2102002-01	2
Audor Pharma	Ureia	PU145	1
Beiersdorf AG	Ureia	14/18-B03-303576	1
Beiersdorf	Ureia	15154112	1
Beyvers/AHD	Ureia	15087104	1
Bombastus	Ureia	11150721	1
Bombastus	Ureia	14107108	1
Bombastus	Ureia	15087107	1
Bombastus	Ureia	15154104	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Ureia	1601044-01	1
Bombastus	Ureia	16107424	2
Bombastus	Ureia	1707015-01	1
Bombastus	Ureia	18023004	1
Bombastus	Ureia	18023010	1
Bombastus	Ureia	18023012	1
Bombastus	Ureia	1804007-01	1
cae	Ureia	16107428	1
Caelo	Ureia		10
Caelo	Ureia	10038587	4
Caelo	Ureia	10038593	1
Caelo	Ureia	100385993	1
Caelo	Ureia	10081208	1
Caelo	Ureia	10116	1
Caelo	Ureia	10169722	1
Caelo	Ureia	10169726	3
Caelo	Ureia	1019E-02544	1
Caelo	Ureia	1061801	1
Caelo	Ureia	107063	1
Caelo	Ureia	10823004	1
Caelo	Ureia	110087-3	1
Caelo	Ureia	1113A-025	1
Caelo	Ureia	11150702	2
Caelo	Ureia	11150703	1
Caelo	Ureia	11150713	1
Caelo	Ureia	11150714	1
Caelo	Ureia	11150721	1
Caelo	Ureia	11150722	3
Caelo	Ureia	11150725	3
Caelo	Ureia	11150736	4
Caelo	Ureia	11150738	1
Caelo	Ureia	1171003	1
Caelo	Ureia	118023004	1
Caelo	Ureia	12111801	4
Caelo	Ureia	12111802	8
Caelo	Ureia	12111803	1
Caelo	Ureia	12111804	4
Caelo	Ureia	12111806	5
Caelo	Ureia	12111807	5
Caelo	Ureia	12111808	9
Caelo	Ureia	12111809	12
Caelo	Ureia	12111810	14
Caelo	Ureia	12111820	11
Caelo	Ureia	12111822	16
Caelo	Ureia	12111823	9
Caelo	Ureia	12111826	6
Caelo	Ureia	12111828	20
Caelo	Ureia	12111834	3
Caelo	Ureia	1211804	1
Caelo	Ureia	1211806	1
Caelo	Ureia	1211808	1
Caelo	Ureia	1211809	1
Caelo	Ureia	1211820	1
Caelo	Ureia	1222	1
Caelo	Ureia	12312478	1
Caelo	Ureia	1234	1
Caelo	Ureia	12345	1
Caelo	Ureia	123456	4
Caelo	Ureia	123566	1
Caelo	Ureia	1236	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ureia	1241017	1
Caelo	Ureia	12L10-N08	3
Caelo	Ureia	13042015B	1
Caelo	Ureia	13062415	1
Caelo	Ureia	1306412	1
Caelo	Ureia	13064201	6
Caelo	Ureia	13064202	12
Caelo	Ureia	13064203	11
Caelo	Ureia	13064206	18
Caelo	Ureia	13064207	18
Caelo	Ureia	13064212	23
Caelo	Ureia	13064213	5
Caelo	Ureia	13064214	13
Caelo	Ureia	13064215	24
Caelo	Ureia	13064217	1
Caelo	Ureia	1306422	1
Caelo	Ureia	13064221	6
Caelo	Ureia	13064223	33
Caelo	Ureia	13064224	2
Caelo	Ureia	13064226	13
Caelo	Ureia	13064227	5
Caelo	Ureia	13064228	23
Caelo	Ureia	13064230	15
Caelo	Ureia	13064231	9
Caelo	Ureia	13064232	17
Caelo	Ureia	13064233	17
Caelo	Ureia	13064236	9
Caelo	Ureia	13064239	2
Caelo	Ureia	13072015B	1
Caelo	Ureia	1317B02-287602	1
Caelo	Ureia	1364212	1
Caelo	Ureia	13E21-N05	1
Caelo	Ureia	14/18-B03-303581	2
Caelo	Ureia	14011513	1
Caelo	Ureia	14064233	1
Caelo	Ureia	1407109	1
Caelo	Ureia	14107101	13
Caelo	Ureia	14107102	27
Caelo	Ureia	14107103	8
Caelo	Ureia	14107108	10
Caelo	Ureia	14107109	21
Caelo	Ureia	14107112	20
Caelo	Ureia	14107113	17
Caelo	Ureia	14107117	10
Caelo	Ureia	14107118	8
Caelo	Ureia	14107119	25
Caelo	Ureia	14107120	10
Caelo	Ureia	14107122	17
Caelo	Ureia	14107424	1
Caelo	Ureia	14107428	1
Caelo	Ureia	14197118	1
Caelo	Ureia	14E07-B05-289706	1
Caelo	Ureia	14E07-B05-293469	1
Caelo	Ureia	14I18-B03	1
Caelo	Ureia	14I18-B03-303581	1
Caelo	Ureia	1501232	1
Caelo	Ureia	1508/104	1
Caelo	Ureia	15087102	8
Caelo	Ureia	15087103	23
Caelo	Ureia	15087104	20

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ureia	15087105	12
Caelo	Ureia	15087107	20
Caelo	Ureia	15087110	26
Caelo	Ureia	151154112	1
Caelo	Ureia	1514107	1
Caelo	Ureia	1514109	1
Caelo	Ureia	1514110	2
Caelo	Ureia	1514112	1
Caelo	Ureia	15145112	1
Caelo	Ureia	1515404	1
Caelo	Ureia	151541	2
Caelo	Ureia	15154101	1
Caelo	Ureia	15154103	51
Caelo	Ureia	15154104	98
Caelo	Ureia	15154107	23
Caelo	Ureia	15154109	10
Caelo	Ureia	15154110	43
Caelo	Ureia	15154111	44
Caelo	Ureia	151541111	1
Caelo	Ureia	15154112	50
Caelo	Ureia	15154113	27
Caelo	Ureia	15154116	16
Caelo	Ureia	15154116I-020117/1	1
Caelo	Ureia	1517E-02544	1
Caelo	Ureia	15299506	1
Caelo	Ureia	16/13-B02-332593	1
Caelo	Ureia	160125/2	1
Caelo	Ureia	1604044-01	1
Caelo	Ureia	160612/3	1
Caelo	Ureia	160620UP	1
Caelo	Ureia	1607406	1
Caelo	Ureia	1607407	1
Caelo	Ureia	1607417	1
Caelo	Ureia	1607422	1
Caelo	Ureia	161017411	1
Caelo	Ureia	1610407	1
Caelo	Ureia	1610426	1
Caelo	Ureia	161072422	1
Caelo	Ureia	16107248	1
Caelo	Ureia	161074	2
Caelo	Ureia	16107404	1
Caelo	Ureia	16107405	13
Caelo	Ureia	16107406	23
Caelo	Ureia	16107407	42
Caelo	Ureia	16107408	2
Caelo	Ureia	16107411	40
Caelo	Ureia	16107412	100
Caelo	Ureia	16107413	11
Caelo	Ureia	16107416	19
Caelo	Ureia	161074165325	1
Caelo	Ureia	16107417	36
Caelo	Ureia	16107417-60717/1	1
Caelo	Ureia	16107418	35
Caelo	Ureia	16107419	26
Caelo	Ureia	16107420	60
Caelo	Ureia	16107422	51
Caelo	Ureia	16107423	12
Caelo	Ureia	16107424	89
Caelo	Ureia	16107425	7
Caelo	Ureia	16107426	27

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ureia	16107427	1
Caelo	Ureia	16107428	31
Caelo	Ureia	16107429	10
Caelo	Ureia	1610743	1
Caelo	Ureia	161107417	1
Caelo	Ureia	161122-1315	1
Caelo	Ureia	16D22-B02-322526	1
Caelo	Ureia	16I13-B02-330166	1
Caelo	Ureia	16I13-B02-332953	1
Caelo	Ureia	17011405	1
Caelo	Ureia	1702023-01	3
Caelo	Ureia	17021601	5
Caelo	Ureia	170509UP/16107407	1
Caelo	Ureia	1707015-01	2
Caelo	Ureia	17101310	1
Caelo	Ureia	17107429	1
Caelo	Ureia	17321206	1
Caelo	Ureia	18012012	1
Caelo	Ureia	1802003	1
Caelo	Ureia	180223003	1
Caelo	Ureia	18023001	18
Caelo	Ureia	18023003	64
Caelo	Ureia	18023003-20180830Ma2	1
Caelo	Ureia	18023004	164
Caelo	Ureia	18023006	74
Caelo	Ureia	18023007	46
Caelo	Ureia	18023007P-190225-12	1
Caelo	Ureia	18023008	1
Caelo	Ureia	18023010	75
Caelo	Ureia	18023011	106
Caelo	Ureia	18023012	113
Caelo	Ureia	18023015	107
Caelo	Ureia	18023016	8
Caelo	Ureia	18023018	55
Caelo	Ureia	18023019	6
Caelo	Ureia	18023022	6
Caelo	Ureia	1802304	1
Caelo	Ureia	1802310	1
Caelo	Ureia	1802401	1
Caelo	Ureia	1802402	1
Caelo	Ureia	18024201	58
Caelo	Ureia	18024202	58
Caelo	Ureia	18024210	1
Caelo	Ureia	1803003	1
Caelo	Ureia	180322H/18024202	1
Caelo	Ureia	1804007-01	1
Caelo	Ureia	18109801	1
Caelo	Ureia	18203012	1
Caelo	Ureia	1823004	1
Caelo	Ureia	1824202	1
Caelo	Ureia	18G04-B03-353339	1
Caelo	Ureia	19016003	1
Caelo	Ureia	19031	1
Caelo	Ureia	19031314	1
Caelo	Ureia	190316001	1
Caelo	Ureia	190316002	9
Caelo	Ureia	190316003	110
Caelo	Ureia	190316003/4520	1
Caelo	Ureia	190316003-1	1
Caelo	Ureia	190316004	103

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ureia	190316005	3
Caelo	Ureia	190316006	43
Caelo	Ureia	19031602	1
Caelo	Ureia	19031603	8
Caelo	Ureia	19031604	86
Caelo	Ureia	19031605	61
Caelo	Ureia	19031606	51
Caelo	Ureia	19031607	4
Caelo	Ureia	19031609	49
Caelo	Ureia	19031610	45
Caelo	Ureia	19031611	7
Caelo	Ureia	19031612	1
Caelo	Ureia	19031614	47
Caelo	Ureia	19031615	58
Caelo	Ureia	19031616	8
Caelo	Ureia	19031616P-200402-3	1
Caelo	Ureia	190318003	1
Caelo	Ureia	190319614	1
Caelo	Ureia	190321604	1
Caelo	Ureia	1903604	1
Caelo	Ureia	19041703	1
Caelo	Ureia	19061615	1
Caelo	Ureia	1908019-01	1
Caelo	Ureia	2/20141507	1
Caelo	Ureia	200001171004	1
Caelo	Ureia	2000011710054	1
Caelo	Ureia	200003817013	1
Caelo	Ureia	200003817016	1
Caelo	Ureia	2000117002	1
Caelo	Ureia	20001171002	10
Caelo	Ureia	20001171003	11
Caelo	Ureia	20001171004	70
Caelo	Ureia	200011711002	1
Caelo	Ureia	200011711004	1
Caelo	Ureia	2000171004	1
Caelo	Ureia	2000381	1
Caelo	Ureia	20003817001	1
Caelo	Ureia	20003817002	28
Caelo	Ureia	20003817004	15
Caelo	Ureia	20003817005	5
Caelo	Ureia	20003817006	7
Caelo	Ureia	20003817008	3
Caelo	Ureia	20003817010	4
Caelo	Ureia	20003817011	16
Caelo	Ureia	20003817012	22
Caelo	Ureia	20003817013	45
Caelo	Ureia	20003817014	7
Caelo	Ureia	20003817015	61
Caelo	Ureia	20003817016	31
Caelo	Ureia	20003817017	1
Caelo	Ureia	2000381705	1
Caelo	Ureia	20003817061	1
Caelo	Ureia	20003817105	1
Caelo	Ureia	2000387004	1
Caelo	Ureia	2001171004	1
Caelo	Ureia	20013100721	1
Caelo	Ureia	20031514	1
Caelo	Ureia	2003817006	1
Caelo	Ureia	200401001	1
Caelo	Ureia	2004010-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ureia	20130912-4	1
Caelo	Ureia	2016142709	1
Caelo	Ureia	20A30-B16-196837	1
Caelo	Ureia	210002313009	1
Caelo	Ureia	2100231008	1
Caelo	Ureia	2100231009	3
Caelo	Ureia	2100231017	1
Caelo	Ureia	2100231300	1
Caelo	Ureia	21002313002	5
Caelo	Ureia	21002313004	41
Caelo	Ureia	21002313005	4
Caelo	Ureia	21002313006	56
Caelo	Ureia	21002313007	35
Caelo	Ureia	21002313008	6
Caelo	Ureia	21002313009	23
Caelo	Ureia	21002313013	2
Caelo	Ureia	21002313014	27
Caelo	Ureia	21002313015	38
Caelo	Ureia	21002313016	4
Caelo	Ureia	21002313017	25
Caelo	Ureia	21003006231	1
Caelo	Ureia	2100313007	1
Caelo	Ureia	210231304	1
Caelo	Ureia	21041802	1
Caelo	Ureia	21051304	1
Caelo	Ureia	2109212544	1
Caelo	Ureia	211100231006	1
Caelo	Ureia	21111806	1
Caelo	Ureia	2116A-02544	1
Caelo	Ureia	22002605001	19
Caelo	Ureia	22002605002	3
Caelo	Ureia	22002605003	10
Caelo	Ureia	22002605005	1
Caelo	Ureia	22002605009	2
Caelo	Ureia	22002605010	3
Caelo	Ureia	2200605001	1
Caelo	Ureia	22111305	1
Caelo	Ureia	230320/2	1
Caelo	Ureia	2324534	1
Caelo	Ureia	2416I-02544	1
Caelo	Ureia	24882000381715	1
Caelo	Ureia	25082015A	1
Caelo	Ureia	26071304	1
Caelo	Ureia	2738	1
Caelo	Ureia	30031304	1
Caelo	Ureia	3012A-02544	1
Caelo	Ureia	3017E-02544	1
Caelo	Ureia	314Q2544	1
Caelo	Ureia	3270	1
Caelo	Ureia	3357	1
Caelo	Ureia	34567890	1
Caelo	Ureia	4013Q2544	1
Caelo	Ureia	4111M-02544	1
Caelo	Ureia	4116M-02544	1
Caelo	Ureia	4517M-02544	1
Caelo	Ureia	4914I-02544	1
Caelo	Ureia	502172207	1
Caelo	Ureia	5061410	1
Caelo	Ureia	5100	1
Caelo	Ureia	5208	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ureia	54215	1
Caelo	Ureia	568900	1
Caelo	Ureia	6101703	1
Caelo	Ureia	62/AKD49	1
Caelo	Ureia	63/AKD4	1
Caelo	Ureia	813051Up	1
Caelo	Ureia	84(18023010)	1
Caelo	Ureia	85(18023012)	2
Caelo	Ureia	88(20003817002)	1
Caelo	Ureia	9031606	1
Caelo	Ureia	9031615	1
Caelo	Ureia	9240908	1
Caelo	Ureia	AKD6	1
Caelo	Ureia	Caelo13064233	1
Caelo	Ureia	P171218UP08/18	1
Caelo	Ureia	Validierungsmessung	1
Caeolo/Gehe	Ureia	16107424	1
Caeolo/Noweda	Ureia	14107112	1
Caeolo/Noweda	Ureia	18023004	1
Caerlo	Ureia	18023018	1
Caesar & Lorenz GmbH	Ureia	15087107	1
Caesar & Lorenz GmbH	Ureia	190316004	1
Caesar & Lorenz GmbH	Ureia	19031604	1
Caesar & Loretz / Gehe	Ureia	16107428	1
Caesar & Loretz /Phönix	Ureia	21002313006	1
Caesar & Loretz GmbH…	Ureia	20003817012	1
Caesar & Loretz GmbH…	Ureia	15154111	1
Caesar & Loretz GmbH…	Ureia	18023010	1
Caesar & Loretz GmbH…	Ureia	19031603	1
Caesar & Loretz GmbH…	Ureia	20003817012	1
Caesar & Loretz GmbH…	Ureia	16107417	1
Caesar & Loretz GmbH…	Ureia	17347901	1
Caesar & Loretz GmbH…	Ureia	18023003	1
Caesar & Loretz GmbH…	Ureia	20003817011	3
Caesar & Loretz GmbH…	Ureia	21002313005	1
Caesar & Loretz GmbH…	Ureia	22002605010	1
Caesar & Loretz GmbH…	Ureia	19031605	1
Caesar & Loretz GmbH…	Ureia	21002313002	1
Caesar & Loretz GmbH…	Ureia	190316003	1
Caesar & Loretz GmbH…	Ureia	19031616	1
Caesar & Loretz GmbH…	Ureia	21002313004	1
Caesar & Loretz GmbH…	Ureia	21002313007	2
Caesar & Loretz GmbH…	Ureia	19031610	1
Caesar & Loretz GmbH…	Ureia	190316003	2
Caesar & Loretz GmbH…	Ureia	21002313007	1
Caesar & Loretz GmbH…	Ureia	20003817015	1
Caesar & Loretz GmbH…	Ureia	11150736	1
Caesar & Loretz GmbH…	Ureia	12111804	1
Caesar & Loretz GmbH…	Ureia	12111810	2
Caesar & Loretz GmbH…	Ureia	12111822	1
Caesar & Loretz GmbH…	Ureia	12111828	2
Caesar & Loretz GmbH…	Ureia	13064206	2
Caesar & Loretz GmbH…	Ureia	13064212	3
Caesar & Loretz GmbH/ AEP	Ureia	20001171004	1
Caesar & Loretz GmbH…	Ureia	19031604	1
Caesar & Loretz GmbH…	Ureia	19031615	1
Caesar & Loretz GmbH…	Ureia	20001171003	1
Caesar & Loretz GmbH…	Ureia	20001171004	1
Caesar & Loretz GmbH…	Ureia	19031605	1
Caesar & Loretz GmbH…	Ureia	19031606	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Ureia	20003817002	1
Caesar & Loretz GmbH...	Ureia	20003817013	1
Caesar & Loretz GmbH...	Ureia	19031610	2
Caesar & Loretz GmbH...	Ureia	20001171003	1
Caesar & Loretz GmbH...	Ureia	21002313014	1
Caesar & Loretz GmbH...	Ureia	19031606	1
Caesar & Loretz GmbH...	Ureia	190316004	1
Caesar & Loretz GmbH...	Ureia	21002313020	1
Caesar & Loretz GmbH...	Ureia	18023015	1
Caesar & Loretz GmbH...	Ureia	19031609	1
Caesar & Loretz GmbH...	Ureia	19031610	1
Caesar & Loretz GmbH/A	Ureia	21002313007	1
Caesar & Loretz GmbH/AHD	Ureia	20003817015	1
Caesar & Loretz GmbH/All	Ureia	190316005	1
Caesar & Loretz GmbH...	Ureia	20003817016	1
Caesar & Loretz GmbH...	Ureia	18023018	1
Caesar & Loretz GmbH...	Ureia	190316004	1
Caesar & Loretz GmbH...	Ureia	19031611	1
Caesar & Loretz GmbH...	Ureia	20003817015	1
Caesar & Loretz GmbH/E	Ureia	19031614	1
Caesar & Loretz GmbH/E	Ureia	20003817015	1
Caesar & Loretz GmbH...	Ureia	18023011	1
Caesar & Loretz GmbH...	Ureia	18023015	1
Caesar & Loretz GmbH...	Ureia	190316004	3
Caesar & Loretz GmbH...	Ureia	19031606	2
Caesar & Loretz GmbH...	Ureia	20003817011	1
Caesar & Loretz GmbH...	Ureia	21002313006	1
Caesar & Loretz GmbH...	Ureia	21002313015	1
Caesar & Loretz GmbH/Gehe	Ureia	18023011	1
Caesar & Loretz GmbH/GEHE	Ureia	18023011	1
Caesar & Loretz GmbH/Gehe	Ureia	190316003	3
Caesar & Loretz GmbH/Gehe	Ureia	190316004	1
Caesar & Loretz GmbH/GEHE	Ureia	190316004	1
Caesar & Loretz GmbH/Gehe	Ureia	190316006	3
Caesar & Loretz GmbH/Gehe	Ureia	19031604	1
Caesar & Loretz GmbH/GEHE	Ureia	19031604	1
Caesar & Loretz GmbH/Gehe	Ureia	19031609	1
Caesar & Loretz GmbH/Gehe	Ureia	19031614	4
Caesar & Loretz GmbH/gehe	Ureia	19031615	1
Caesar & Loretz GmbH/GEHE	Ureia	19031615	1
Caesar & Loretz GmbH/GEHE	Ureia	20001171003	2
Caesar & Loretz GmbH/Gehe	Ureia	20001171004	1
Caesar & Loretz GmbH/GEHE	Ureia	20001171004	2
Caesar & Loretz GmbH/Gehe	Ureia	20003817006	2
Caesar & Loretz GmbH/GEHE	Ureia	20003817015	1
Caesar & Loretz GmbH/Gehe	Ureia	20003817016	1
Caesar & Loretz GmbH/Gehe	Ureia	21002313004	2
Caesar & Loretz GmbH/Gehe	Ureia	22002605001	1
Caesar & Loretz GmbH...	Ureia	20003817008	1
Caesar & Loretz GmbH...	Ureia	18023019	1
Caesar & Loretz GmbH...	Ureia	190316003	1
Caesar & Loretz GmbH...	Ureia	21002313014	1
Caesar & Loretz GmbH...	Ureia	20003817016	1
Caesar & Loretz GmbH...	Ureia	190316002	1
Caesar & Loretz GmbH...	Ureia	19031603	1
Caesar & Loretz GmbH...	Ureia	19031610	1
Caesar & Loretz GmbH...	Ureia	19031616	1
Caesar & Loretz GmbH/kehr	Ureia	18023007	2
Caesar & Loretz GmbH/Kehr	Ureia	18023015	1
Caesar & Loretz GmbH/Kehr	Ureia	18023019	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Kehr	Ureia	190316002	1
Caesar & Loretz GmbH/Kehr	Ureia	190316003	2
Caesar & Loretz GmbH/Kehr	Ureia	19031616	1
Caesar & Loretz GmbH/Kehr	Ureia	22002605001	2
Caesar & Loretz GmbH...	Ureia	190316004	2
Caesar & Loretz GmbH...	Ureia	19031615	1
Caesar & Loretz GmbH...	Ureia	20001171004	2
Caesar & Loretz GmbH...	Ureia	19031614	1
Caesar & Loretz GmbH...	Ureia	20003817016	1
Caesar & Loretz GmbH...	Ureia	190316004	1
Caesar & Loretz GmbH...	Ureia	190316006	1
Caesar & Loretz GmbH...	Ureia	19031615	1
Caesar & Loretz GmbH...	Ureia	20001171004	1
Caesar & Loretz GmbH...	Ureia	21002313006	1
Caesar & Loretz GmbH/Phoe	Ureia	20003817012	1
Caesar & Loretz GmbH...	Ureia	190316006	1
Caesar & Loretz GmbH...	Ureia	19031606	1
Caesar & Loretz GmbH...	Ureia	20003817005	1
Caesar & Loretz GmbH...	Ureia	20003817015	1
Caesar & Loretz GmbH...	Ureia	21002313015	2
Caesar & Loretz GmbH...	Ureia	18023006	1
Caesar & Loretz GmbH...	Ureia	190316003	1
Caesar & Loretz GmbH...	Ureia	190316004	1
Caesar & Loretz GmbH...	Ureia	190316006	1
Caesar & Loretz GmbH...	Ureia	19031603	2
Caesar & Loretz GmbH...	Ureia	19031611	1
Caesar & Loretz GmbH...	Ureia	19031615	1
Caesar & Loretz GmbH...	Ureia	20001171003	1
Caesar & Loretz GmbH...	Ureia	20003817004	1
Caesar & Loretz GmbH...	Ureia	20003817015	4
Caesar & Loretz GmbH...	Ureia	21002313004	1
Caesar & Loretz GmbH...	Ureia	21002313007	2
Caesar & Loretz GmbH...	Ureia	21002313009	1
Caesar & Loretz GmbH...	Ureia	21002313015	1
Caesar & Loretz GmbH...	Ureia	22002605010	1
Caesar & Loretz GmbH...	Ureia	23001146002	2
Caesar & Loretz GmbH...	Ureia	190316003	1
Caesar & Loretz GmbH...	Ureia	190316004	2
Caesar & Loretz GmbH...	Ureia	190316006	1
Caesar & Loretz GmbH...	Ureia	19031604	1
Caesar & Loretz GmbH...	Ureia	19031606	1
Caesar & Loretz GmbH...	Ureia	19031615	1
Caesar & Loretz GmbH...	Ureia	20001171004	1
Caesar & Loretz GmbH...	Ureia	20003817006	1
Caesar & Loretz GmbH...	Ureia	20003817015	2
Caesar & Loretz GmbH...	Ureia	21002313007	3
Caesar & Loretz GmbH...	Ureia	22002605001	1
Caesar & Loretz GmbH...	Ureia	AP210316-01	1
Caesar & Loretz GmbH	Ureia	12111822	1
Caesar & Loretz GmbH	Ureia	13064206	1
Caesar & Loretz GmbH	Ureia	1306421	1
Caesar & Loretz GmbH	Ureia	13064223	1
Caesar & Loretz GmbH	Ureia	15087103	1
Caesar & Loretz GmbH	Ureia	15087105	1
Caesar & Loretz GmbH	Ureia	15154104	1
Caesar & Loretz GmbH	Ureia	16107411	1
Caesar & Loretz GmbH	Ureia	16107417	1
Caesar & Loretz GmbH	Ureia	16107419	1
Caesar & Loretz GmbH	Ureia	18023004	2
Caesar & Loretz GmbH	Ureia	18023006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ureia	18023007	1
Caesar & Loretz GmbH	Ureia	18023008	1
Caesar & Loretz GmbH	Ureia	18023010	2
Caesar & Loretz GmbH	Ureia	18023011	6
Caesar & Loretz GmbH	Ureia	18023012	9
Caesar & Loretz GmbH	Ureia	18023013	1
Caesar & Loretz GmbH	Ureia	18023015	23
Caesar & Loretz GmbH	Ureia	18023016	1
Caesar & Loretz GmbH	Ureia	18023018	8
Caesar & Loretz GmbH	Ureia	18023019	2
Caesar & Loretz GmbH	Ureia	18023022	1
Caesar & Loretz GmbH	Ureia	18024201	1
Caesar & Loretz GmbH	Ureia	190316002	6
Caesar & Loretz GmbH	Ureia	190316003	26
Caesar & Loretz GmbH	Ureia	190316004	44
Caesar & Loretz GmbH	Ureia	190316005	9
Caesar & Loretz GmbH	Ureia	190316006	15
Caesar & Loretz GmbH	Ureia	19031602	1
Caesar & Loretz GmbH	Ureia	19031603	6
Caesar & Loretz GmbH	Ureia	19031604	21
Caesar & Loretz GmbH	Ureia	19031605	14
Caesar & Loretz GmbH	Ureia	19031606	11
Caesar & Loretz GmbH	Ureia	19031607	1
Caesar & Loretz GmbH	Ureia	19031608	1
Caesar & Loretz GmbH	Ureia	19031609	9
Caesar & Loretz GmbH	Ureia	19031610	13
Caesar & Loretz GmbH	Ureia	19031611	4
Caesar & Loretz GmbH	Ureia	19031612	3
Caesar & Loretz GmbH	Ureia	19031614	16
Caesar & Loretz GmbH	Ureia	19031615	20
Caesar & Loretz GmbH	Ureia	19031616	8
Caesar & Loretz GmbH	Ureia	19032609	1
Caesar & Loretz GmbH	Ureia	20000092002	1
Caesar & Loretz GmbH	Ureia	20001171002	2
Caesar & Loretz GmbH	Ureia	20001171003	9
Caesar & Loretz GmbH	Ureia	20001171004	32
Caesar & Loretz GmbH	Ureia	2000171004	1
Caesar & Loretz GmbH	Ureia	20003817002	14
Caesar & Loretz GmbH	Ureia	20003817004	3
Caesar & Loretz GmbH	Ureia	20003817005	1
Caesar & Loretz GmbH	Ureia	20003817006	4
Caesar & Loretz GmbH	Ureia	20003817008	2
Caesar & Loretz GmbH	Ureia	20003817010	4
Caesar & Loretz GmbH	Ureia	20003817011	3
Caesar & Loretz GmbH	Ureia	20003817012	6
Caesar & Loretz GmbH	Ureia	20003817013	12
Caesar & Loretz GmbH	Ureia	20003817014	2
Caesar & Loretz GmbH	Ureia	20003817015	28
Caesar & Loretz GmbH	Ureia	20003817016	10
Caesar & Loretz GmbH	Ureia	21002313001	2
Caesar & Loretz GmbH	Ureia	21002313002	2
Caesar & Loretz GmbH	Ureia	21002313004	12
Caesar & Loretz GmbH	Ureia	21002313005	2
Caesar & Loretz GmbH	Ureia	21002313006	18
Caesar & Loretz GmbH	Ureia	21002313007	23
Caesar & Loretz GmbH	Ureia	21002313008	7
Caesar & Loretz GmbH	Ureia	21002313009	8
Caesar & Loretz GmbH	Ureia	21002313013	1
Caesar & Loretz GmbH	Ureia	21002313014	15
Caesar & Loretz GmbH	Ureia	21002313015	21

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ureia	21002313016	1
Caesar & Loretz GmbH	Ureia	21002313017	6
Caesar & Loretz GmbH	Ureia	220002605001	1
Caesar & Loretz GmbH	Ureia	22002605001	10
Caesar & Loretz GmbH	Ureia	22002605003	2
Caesar & Loretz GmbH	Ureia	22002605009	1
Caesar & Loretz GmbH	Ureia	22002605010	1
Caesar & Loretz GmbH7Gehe	Ureia	20003817015	1
Caesar & Loretz Hild...	Ureia	19031614	1
Caesar & Loretz Hilden	Ureia	18023012	1
Caesar & Loretz Hilden	Ureia	190316004	1
Caesar & Loretz Hilden	Ureia	19031609	1
Caesar & Loretz/AHD	Ureia	18023007	2
Caesar & Loretz/Gehe	Ureia	19031606	1
Caesar & Loretz/Geil...	Ureia	190316003	1
Caesar & Loretz	Ureia	16107426	1
Caesar & Loretz	Ureia	18023004	2
Caesar & Loretz	Ureia	18024201	1
Caesar & Loretz	Ureia	20003817002	1
Caesar & Loretz	Ureia	20003817015	1
Caesar & Loretz	Ureia	21002313006	1
Caesar &Loretz GmbH	Ureia	13064203	1
Caesar u Loretz	Ureia	12111828	1
Caesar und Loretz Gm...	Ureia	18023015	1
Caesar und Loretz GmbH	Ureia	20001171004	1
Caesar und Loretz	Ureia	16107420	1
Caesar&Loretz GmbH /Anzag	Ureia	14107113	1
Caesar&Loretz GmbH /Anzag	Ureia	15087110	1
Caesar&Loretz GmbH D...	Ureia	12111808	2
Caesar&Loretz GmbH,P...	Ureia	16107411	1
Caesar&Loretz GmbH/ ...	Ureia	18023001	2
Caesar&Loretz GmbH/Anzag	Ureia	13064217	1
Caesar&Loretz GmbH/Anzag	Ureia	13064231	1
Caesar&Loretz GmbH	Ureia	14107101	1
Caesar&Loretz GmbH	Ureia	15154111	1
Caesar&Loretz GmbH	Ureia	16107417	1
Caesar&Loretz GmbH	Ureia	20003817013	1
Caesar&Loretz GmbH	Ureia	21002313004	1
Caesar&loretz,Anzag	Ureia	11150738	1
Caesar&loretz,Phoenix	Ureia	11150713	1
Caesar&loretz,Phoenix	Ureia	12111806	3
Caesar&Loretz/Caesar...	Ureia	15154104	1
Caesar&Loretz	Ureia	16107428	1
Caesar/Lorenz	Ureia	12111822	1
Caesar/Noweda	Ureia	12111823	1
Caesar/Noweda	Ureia	13064208	1
CaesarLoretz/Gehe	Ureia	16107407	1
CaesarLoretz/Gehe	Ureia	16107418	1
CaesarLoretz/Gehe	Ureia	18023004	1
Caeser & Loretz GmbH/AEP	Ureia	21002313006	1
Caeser / Gehe	Ureia	15154109	1
Caeser und Loretz GmbH	Ureia	18023018	1
Caleo/Noveda	Ureia	20003817011	1
Caleo	Ureia	18023018	1
Calo/AHD	Ureia	15154104	1
Castor/Phönix	Ureia	15154104	1
Cealo/AHD	Ureia	16107417	1
Cealo/Gehe	Ureia	20003817015	1
Cealo/Jenne	Ureia	220321(21002313004)	1
Cealo/Phoenix	Ureia	18023018	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo/Phönix	Ureia	13064231	1
Cealo/Sanacorp	Ureia	1804007-01	1
Cealo	Ureia	16107416	1
Cealo	Ureia	190316003	3
Ceasar & Loretz GmbH...	Ureia	16107422	2
Cordes/Noweda	Ureia	17021601	1
Dan Pharma	Ureia	D08118	1
Delta	Ureia	18023004	1
Dr. August Wolff	Ureia	13E17N02	1
Dr.Wolff	Ureia	1234567	1
Ebert & Jacobi	Ureia	15154111	1
Eur	Ureia	1707015-01	1
EurHo/ Noweda 11.10.18	Ureia	1804007-01	1
EuRho/Noweda	Ureia	1707015-01	1
EuRho/Phönix	Ureia	2102002-01	1
EuRho	Ureia	1212007-01	1
Eurho	Ureia	1404024-01	1
EuRho	Ureia	150304201	1
EuRho	Ureia	1702023-01	1
EuRho	Ureia	1707015-01	1
EuRho	Ureia	2004010-01	1
Euro / AHD	Ureia	1804007-01	1
Euro OTC	Ureia		12
Euro OTC	Ureia	1008016-01	1
Euro OTC	Ureia	1110023-01	1
Euro OTC	Ureia	1212007-01	6
Euro OTC	Ureia	1212007-02	3
Euro OTC	Ureia	13064239	1
Euro OTC	Ureia	1404024-01	12
Euro OTC	Ureia	14107101	2
Euro OTC	Ureia	14107108	1
Euro OTC	Ureia	150304201	1
Euro OTC	Ureia	1503042-01	26
Euro OTC	Ureia	1515404	1
Euro OTC	Ureia	15154103	2
Euro OTC	Ureia	15154104	3
Euro OTC	Ureia	15154107	2
Euro OTC	Ureia	160104401	1
Euro OTC	Ureia	1601044-01	29
Euro OTC	Ureia	160404401	2
Euro OTC	Ureia	1604044-01	30
Euro OTC	Ureia	16107411	1
Euro OTC	Ureia	16107412	3
Euro OTC	Ureia	16107428	1
Euro OTC	Ureia	16I13-B02-332953	1
Euro OTC	Ureia	1702023	1
Euro OTC	Ureia	170202301	4
Euro OTC	Ureia	1702023-01	30
Euro OTC	Ureia	170701501	4
Euro OTC	Ureia	1707015-01	41
Euro OTC	Ureia	18023006	1
Euro OTC	Ureia	18023010	1
Euro OTC	Ureia	18023012	1
Euro OTC	Ureia	18023015	1
Euro OTC	Ureia	18024201	1
Euro OTC	Ureia	180400701	1
Euro OTC	Ureia	1804007-01	57
Euro OTC	Ureia	1804007-02	9
Euro OTC	Ureia	1804007-1	1
Euro OTC	Ureia	18040701	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Ureia	1811012_01	1
Euro OTC	Ureia	181101201	1
Euro OTC	Ureia	1811012-01	67
Euro OTC	Ureia	18110-12-01	1
Euro OTC	Ureia	18A24-B07-349015	1
Euro OTC	Ureia	19031611	1
Euro OTC	Ureia	190801601	2
Euro OTC	Ureia	1908016-01	41
Euro OTC	Ureia	1908016-16	1
Euro OTC	Ureia	1915M-02544	1
Euro OTC	Ureia	20003817010	1
Euro OTC	Ureia	200401001	2
Euro OTC	Ureia	2004010-01	35
Euro OTC	Ureia	2004010-02	8
Euro OTC	Ureia	2004010-10	1
Euro OTC	Ureia	21002313009	1
Euro OTC	Ureia	2101002-02	1
Euro OTC	Ureia	210200-01	1
Euro OTC	Ureia	2102002	1
Euro OTC	Ureia	2102002-01	31
Euro OTC	Ureia	2102002-02	6
Euro OTC	Ureia	2102002-2	1
Euro OTC	Ureia	2109001-01	16
Euro OTC	Ureia	2205037	1
Euro OTC	Ureia	2205037-01	24
Euro OTC	Ureia	2205037-02	1
Euro OTC	Ureia	220537-01	1
Euro OTC	Ureia	72/14	1
Euro OTC	Ureia	hcvovo	1
Euro OTC	Ureia	UP250171017	1
Euro OTC	Ureia	V038-2017	1
Euro OTC	Ureia	V076-2016	1
Euro OTC	Ureia	V081-2018	3
Euro/Sanacorp	Ureia	1707015-01	1
Euro/Sanacorp	Ureia	1804007-01	1
Euro/Sanacorp	Ureia	1908016-01	2
Fagon/Noweda	Ureia	18A24-B07-351975	1
Fagon/Noweda	Ureia	19G11-B01	1
Fagon/Noweda	Ureia	B01-2014803	1
Fagon/Noweda	Ureia	B16-1928504	1
Fagon/Noweda	Ureia	V016-2019	1
Fagron	Ureia	118900-0001	1
Fagron	Ureia	11C25-N01	1
Fagron	Ureia	11F24-N16	1
Fagron	Ureia	11H01-N08	2
Fagron	Ureia	1211822	1
Fagron	Ureia	1232255144	1
Fagron	Ureia	123456	1
Fagron	Ureia	12C20-N05	1
Fagron	Ureia	12F25-N05	5
Fagron	Ureia	12I04-N06	1
Fagron	Ureia	12l04-N06	1
Fagron	Ureia	12l10-n08	1
Fagron	Ureia	12L10-N08	5
Fagron	Ureia	13/17-1302-287602	1
Fagron	Ureia	13D03-N01	9
Fagron	Ureia	13D03-NO01	1
Fagron	Ureia	13E17-N02	1
Fagron	Ureia	13E21-N05	2
Fagron	Ureia	13J17-B02	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ureia	13J17-B02-287602	2
Fagron	Ureia	13J17B02-287604	1
Fagron	Ureia	13J17-B02-287604	5
Fagron	Ureia	13L20B03	1
Fagron	Ureia	13L20-B03_289708	1
Fagron	Ureia	13L20-B03-289708	6
Fagron	Ureia	14/18-B03-303576	2
Fagron	Ureia	14/18B03303581	1
Fagron	Ureia	14/18-B03-303581	7
Fagron	Ureia	14107117	1
Fagron	Ureia	1418b03303581	1
Fagron	Ureia	1418B03303581	1
Fagron	Ureia	1418-B03-303581	1
Fagron	Ureia	14E07B05	3
Fagron	Ureia	14E07-B05	8
Fagron	Ureia	14E07-B05-289706	1
Fagron	Ureia	14E07B05293469	1
Fagron	Ureia	14E07-B05-293469	9
Fagron	Ureia	14E-07-B05-293469	1
Fagron	Ureia	14E07-B05-297165	4
Fagron	Ureia	14E07-B05-297167	6
Fagron	Ureia	14E07-B07-293469	1
Fagron	Ureia	14E8900-0001	1
Fagron	Ureia	14I18-B03	4
Fagron	Ureia	14I18-B03-303576	7
Fagron	Ureia	14I18-B03-303581	3
Fagron	Ureia	14l18-B03	1
Fagron	Ureia	14l18-B03-0303581	1
Fagron	Ureia	15087104	1
Fagron	Ureia	15154104	2
Fagron	Ureia	15154112	1
Fagron	Ureia	16/13-B02	1
Fagron	Ureia	16/13-B02-330166	2
Fagron	Ureia	16/13-B02-332953	2
Fagron	Ureia	1607417	1
Fagron	Ureia	16107407	1
Fagron	Ureia	16107418	1
Fagron	Ureia	16107422	1
Fagron	Ureia	1613-B02-328152	2
Fagron	Ureia	1613b02332953	1
Fagron	Ureia	16D22-802-326481	1
Fagron	Ureia	16D22-B02	3
Fagron	Ureia	16D22-B02-3221532	1
Fagron	Ureia	16D22-B02-322426	1
Fagron	Ureia	16D22-B02-322526	6
Fagron	Ureia	16D22-B02-322532	5
Fagron	Ureia	16D22B02326481	1
Fagron	Ureia	16D22-B02-326481	9
Fagron	Ureia	16D22-B02-36481	1
Fagron	Ureia	16I13-B02	1
Fagron	Ureia	16I13-B02-328152	3
Fagron	Ureia	16I13-B02-330166	4
Fagron	Ureia	16l13-B02-332953	2
Fagron	Ureia	1707015-01	1
Fagron	Ureia	17D20-B01-335312	1
Fagron	Ureia	17H16-B01	3
Fagron	Ureia	17H16-B01-340516	1
Fagron	Ureia	17H16-B01-342080	4
Fagron	Ureia	18023006	1
Fagron	Ureia	18023012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ureia	18023015	2
Fagron	Ureia	18024202	1
Fagron	Ureia	18A24-B07	3
Fagron	Ureia	18A24-B07-346692	5
Fagron	Ureia	18A24-B07-347410	1
Fagron	Ureia	18A24-B07-3490	1
Fagron	Ureia	18A24-B07-349015	4
Fagron	Ureia	18A24-B07-351975	8
Fagron	Ureia	18A24-B07-352707	3
Fagron	Ureia	18-B03-303581	1
Fagron	Ureia	18G04-B03	1
Fagron	Ureia	18G04-B03-353339	4
Fagron	Ureia	18G04-B03-35339	1
Fagron	Ureia	18G04-B03-355378	1
Fagron	Ureia	18G04-B03-355387	3
Fagron	Ureia	19011-B01-194615	1
Fagron	Ureia	19E07-B16-162854	2
Fagron	Ureia	19E07-B16-190548	3
Fagron	Ureia	19e07-b16-192854	1
Fagron	Ureia	19E07B16192854	1
Fagron	Ureia	19E07-B16-192854	13
Fagron	Ureia	19G11_B01_192855	1
Fagron	Ureia	19G11-B01_194615	1
Fagron	Ureia	19G11-B01-194615	13
Fagron	Ureia	20003817015	1
Fagron	Ureia	2014162937	3
Fagron	Ureia	2016142709	4
Fagron	Ureia	2018163455	1
Fagron	Ureia	20A30-B16	2
Fagron	Ureia	20A30-B16-1968307	1
Fagron	Ureia	20A30-b16-196837	1
Fagron	Ureia	20A30-B16-196837	7
Fagron	Ureia	20A30-B16-196838	2
Fagron	Ureia	20E07-801-201907	1
Fagron	Ureia	20E07-B01	3
Fagron	Ureia	20E07-B01-201455	4
Fagron	Ureia	20E07-B01-201483	7
Fagron	Ureia	20E07B01201907	2
Fagron	Ureia	20E07-B01-201907	9
Fagron	Ureia	211120-B02	1
Fagron	Ureia	21C16-802	1
Fagron	Ureia	21C16-B02	3
Fagron	Ureia	21C16-B02_210554	1
Fagron	Ureia	21C16-B02-210554	3
Fagron	Ureia	21C16-B02-210584	3
Fagron	Ureia	21C16B02214451	1
Fagron	Ureia	21C16-B02-214451	5
Fagron	Ureia	21C16-B02-215566	10
Fagron	Ureia	21C16-B02-215659	2
Fagron	Ureia	21L08-B04-219541	1
Fagron	Ureia	2205037	1
Fagron	Ureia	235/12I04-N06	1
Fagron	Ureia	2OE07B01201483	1
Fagron	Ureia	3613M-02544	1
Fagron	Ureia	7L17-NO1	1
Fagron	Ureia	9K27-M01	1
Fagron	Ureia	B01-2019007	1
Fagron	Ureia	B02-2105504	2
Fagron	Ureia	B03-303581	1
Fagron	Ureia	V018-2021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ureia	V041-2020	2
Fagron	Ureia	V073-2019	1
Fargon/Alliance HC	Ureia	14E07-B05-293469	1
Fargon	Ureia	14e07-b05-297165	1
Fiebig	Ureia	15087103	1
Fiebig	Ureia	15154112	1
Fiebig	Ureia	16107411	1
Fiebig	Ureia	16107417	1
Fiebig	Ureia	16107425	1
Fiebig	Ureia	16107428	1
Fiebig	Ureia	18023004	1
Fiebig	Ureia	18023010	1
Fiebig	Ureia	18023011	2
Fiebig	Ureia	18023018	2
Fiebig	Ureia	18024201	1
Finteler Apotheke	Ureia	16107417	1
Finze	Ureia	1264	1
Gatt-Koller	Ureia	1800697	1
Gatt-Koller	Ureia	1803268	3
Gehe am 11.10.2017	Ureia	16107419	1
Gehe amax	Ureia	16107417	1
Gehe amax	Ureia	16107422	1
Gehe amax	Ureia	18023006	1
Gehe amax	Ureia	190316003	1
Gehe amax	Ureia	19031614	1
Gehe,05.04.17, 5,30EUR	Ureia	16107412	1
Gehe/Fragon	Ureia	16D22-B02-326481	1
Gehe	Ureia	10038593	1
Gehe	Ureia	12111808	1
Gehe	Ureia	12111810	1
Gehe	Ureia	12111822	1
Gehe	Ureia	12111826	1
Gehe	Ureia	13064232	1
Gehe	Ureia	14107112	1
Gehe	Ureia	14107122	1
Gehe	Ureia	15087103	1
Gehe	Ureia	15087107	2
Gehe	Ureia	15154103	1
Gehe	Ureia	15154112	1
Gehe	Ureia	16107411	2
Gehe	Ureia	16107412	3
GEHE	Ureia	16107412	1
GEHE	Ureia	16107416	1
Gehe	Ureia	16107417	1
Gehe	Ureia	16107419	1
Gehe	Ureia	16107422	3
GEHE	Ureia	16107422	1
gehe	Ureia	16107425	1
Gehe	Ureia	16107425	1
Gehe	Ureia	16107428	1
Gehe	Ureia	18023004	3
GEHE	Ureia	18023006	1
GEHE	Ureia	18023007	1
Gehe	Ureia	18023011	3
gehe	Ureia	18023012	1
Gehe	Ureia	18023012	2
Gehe	Ureia	18023015	2
Gehe	Ureia	18023018	1
gehe	Ureia	18024201	1
Gehe	Ureia	18024202	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Ureia	1804007-01	1
Gehe	Ureia	190316002	2
Gehe	Ureia	190316004	1
Gehe	Ureia	19031604	2
Gehe	Ureia	19031606	1
Gehe	Ureia	21002313006	1
Gehe	Ureia	21002313014	1
Gehe	Ureia	210200201	1
GEHE	Ureia	2102313014	1
Gehe	Ureia	21C16-B02	1
Gehe	Ureia	22002605003	1
Gehe	Ureia	22002605010	1
GEHE	Ureia	2205037-02	1
Gehe	Ureia	23001146001	3
Gehe	Ureia	2301020-01	2
Gehe	Ureia	fgjhghk	1
Geilenkirchen	Ureia	18023011	1
Geilenkirchen	Ureia	18023015	1
Gutenberg-Apotheke	Ureia		1
Gutenberg-Apotheke	Ureia	13064227	1
Hänseler	Ureia		3
Harnstoff	Ureia	20003817016	1
Hirsch	Ureia	810811	1
Ichthyol/Noweda	Ureia		1
Ichthyol/Phoenix	Ureia	15154104	1
ichtxol-Gesellschaft…	Ureia	18023010	2
Infectopharm/Phönix	Ureia	18023011	1
Jenne 15.11.21, 4,79EUR	Ureia	211125	1
Jenne	Ureia	18023018	1
Jenne	Ureia	23001146001	2
Kehr	Ureia	16107418	1
Kehr	Ureia	1802007	1
Kehr	Ureia	18023004	1
Kehr	Ureia	21C16-B02-215566	1
Kehr	Ureia	22002605001	1
Kehr	Ureia	22002605011	1
Kehr	Ureia	2205037-02	1
Kehr	Ureia	23001146001	1
Kirsch Pharma GmbH/Noweda	Ureia	14E07-B05-293469	1
Kirsch Pharma	Ureia	18A24B07346692	1
Krieger	Ureia	15154110	1
krieger	Ureia	19031604	1
Krieger	Ureia	19031610	2
L10	Ureia	21C16-B02	1
L12	Ureia	16107418	1
L30	Ureia	16107407	1
L30	Ureia	16107424	1
L30	Ureia	18023011	1
Laborchemie Apolda/J…	Ureia	12345	1
Lamotte	Ureia	19031611	1
Löns Apotheke	Ureia	20349	1
Löns Apotheke	Ureia	40003	1
Nachprüfung	Ureia	2082019-12	1
Nachprüfung	Ureia	iu98769879	1
Noveda	Ureia	19031610	1
Noveda	Ureia	20001171004	1
Noweda 02.08.2019	Ureia	18023018	1
Noweda 02.09.2019	Ureia	18023019	1
Noweda/KremerGmbH	Ureia	13064201	1
Noweda	Ureia	11150714	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Ureia	13064223	1
Noweda	Ureia	14107101	1
Noweda	Ureia	15154110	1
Noweda	Ureia	15154112	1
Noweda	Ureia	16107416	1
Noweda	Ureia	16107419	3
Noweda	Ureia	16107422	1
Noweda	Ureia	18023001	2
Noweda	Ureia	18023004	4
Noweda	Ureia	18023012	1
Noweda	Ureia	18023015	3
Noweda	Ureia	18024201	1
Noweda	Ureia	18024202	2
Noweda	Ureia	19031604	1
Noweda	Ureia	19031609	1
Noweda	Ureia	19031611	1
Noweda	Ureia	20003817004	1
Noweda	Ureia	2003817015	1
Noweda	Ureia	20E07-B01-201907	1
Noweda	Ureia	21002313015	1
Noweda	Ureia	21002313017	2
Noweda	Ureia	210200-01	1
Noweda	Ureia	22002605009	4
NOWEDA	Ureia	22002605009	1
Noweda	Ureia	22002605010	3
Noweda	Ureia	2205037-01	1
Noweda	Ureia	2205037-02	1
Noweda	Ureia	2301020-01	1
Noweda	Ureia	23C21-B01-228853	2
Noweda	Ureia	4109M-02544	1
Pala	Ureia	18G04-B03-353339	1
Ph.Eur.7.0	Ureia	14107109	1
PHOENIX 02.05.2014	Ureia	13J17-B02-287602	2
Phoenix 11.09.2017	Ureia	16107419	1
Phoenix 17.2.2014	Ureia	13064227	1
Phoenix 20.07.2019 4,30EUR	Ureia	18023018	1
PHOENIX 29.08.2014	Ureia		1
Phoenix 31.07.19	Ureia	18023001	1
Phoenix	Ureia	13064231	1
Phoenix	Ureia	15154113	1
Phoenix	Ureia	16107411	1
Phoenix	Ureia	16107420	1
Phoenix	Ureia	16107424	1
Phoenix	Ureia	16107428	1
Phoenix	Ureia	18023004	2
Phoenix	Ureia	18023006	2
Phoenix	Ureia	18023012	1
Phoenix	Ureia	18024201	2
Phoenix	Ureia	190316004	1
Phoenix	Ureia	19031605	1
Phoenix	Ureia	19031615	1
Phoenix	Ureia	20001171004	1
Phoenix	Ureia	20002817013	1
Phoenix	Ureia	20003817002	1
Phoenix	Ureia	20003817006	1
Phoenix	Ureia	20003817012	2
Phoenix	Ureia	21002313014	1
Phoenix	Ureia	22002605001	1
Phoenix	Ureia	23001146002	3
Phoenix	Ureia	23003219012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Ureia	3201	1
Phönix Gotha	Ureia	1212007-01	1
Phönix Gotha	Ureia	13064202	1
Phönix Gotha	Ureia	1404024-01	1
Phönix Gotha	Ureia	16107417	2
Phönix Gotha	Ureia	V096/2012	1
Phönix, Caesar&Loret…	Ureia	190316004	3
Phönix/Gehe	Ureia	18024201	2
Phönix	Ureia	1190316004	1
Phönix	Ureia	12111822	1
Phönix	Ureia	123456	1
Phönix	Ureia	13064207	1
Phönix	Ureia	13064215	1
Phönix	Ureia	13064223	1
Phönix	Ureia	13064236	1
Phönix	Ureia	14107109	1
Phönix	Ureia	15087110	1
phönix	Ureia	15154103	2
phönix	Ureia	15154111	1
phönix	Ureia	15154112	2
Phönix	Ureia	15154113	1
phönix	Ureia	16107412	2
Phönix	Ureia	16107412	2
Phönix	Ureia	16107419	1
phönix	Ureia	16107420	1
Phönix	Ureia	16107424	1
Phönix	Ureia	17H16-B01-342080	1
PHÖNIX	Ureia	18023001	1
Phönix	Ureia	18023003	2
Phönix	Ureia	18023004	1
Phönix	Ureia	18023006	1
Phönix	Ureia	18023010	1
Phönix	Ureia	18023011	1
Phönix	Ureia	18023015	1
Phönix	Ureia	18023018	2
Phönix	Ureia	18024201	1
Phönix	Ureia	190316006	1
Phönix	Ureia	19031604	2
Phönix	Ureia	19031614	2
Phönix	Ureia	19031615	1
PHÖNIX	Ureia	19031615	1
Phönix	Ureia	1908016-01	1
Phönix	Ureia	20001171004	2
Phönix	Ureia	20003817002	1
Phönix	Ureia	20003817012	1
PHÖNIX	Ureia	20003817015	1
Phönix	Ureia	2004010-01	1
Phönix	Ureia	2100231015	1
Phönix	Ureia	2102002-01	1
PHönix	Ureia	2102002-01	1
Phönix	Ureia	22002605001	1
phönix	Ureia	22002605003	1
Phönix	Ureia	22002605003	1
Phönix	Ureia	22002605010	1
Phönix	Ureia	23001146002	1
Phönix	Ureia	2300114601	1
Phönix	Ureia	UP11	1
Phöpnix	Ureia	20003817015	1
Px/Phoenix	Ureia	18023004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Raben-Apotheke Mildenau	Ureia	13J17-B02-287604	2
Raben-Apotheke Mildenau	Ureia	13J17-Bo2-287604	1
Röntgen	Ureia	1811012-01	1
Röntgen	Ureia	190316003	1
Röntgen	Ureia	20003817103	1
sanacorb	Ureia	16107424	1
Sanacorp Verbund	Ureia	21C16-B02-214451	2
Sanacorp	Ureia	1110023-01	1
Sanacorp	Ureia	12111808	2
Sanacorp	Ureia	12111810	1
Sanacorp	Ureia	12111820	1
Sanacorp	Ureia	1212007	1
Sanacorp	Ureia	13064203	1
Sanacorp	Ureia	13064212	1
Sanacorp	Ureia	13064223	1
Sanacorp	Ureia	1405028-01	1
Sanacorp	Ureia	14107102	1
Sanacorp	Ureia	14107112	1
Sanacorp	Ureia	14107113	1
Sanacorp	Ureia	16107417	1
Sanacorp	Ureia	16107418	2
Sanacorp	Ureia	16107423	1
Sanacorp	Ureia	16D22-B02	1
Sanacorp	Ureia	1707015-01	2
Sanacorp	Ureia	18023004	2
Sanacorp	Ureia	18023007	1
Sanacorp	Ureia	18023011	1
Sanacorp	Ureia	18024202	1
Sanacorp	Ureia	1804007-01	2
Sanacorp	Ureia	1811012-01	1
Sanacorp	Ureia	190316002	1
Sanacorp	Ureia	19031604	1
Sanacorp	Ureia	19031609	2
Sanacorp	Ureia	19031610	1
Sanacorp	Ureia	19031615	1
Sanacorp	Ureia	1908016-01	1
Sanacorp	Ureia	19E07-B16-192854	3
Sanacorp	Ureia	20003817015	1
Sanacorp	Ureia	2004010-01	2
Sanacorp	Ureia	20A30-B16-196837	1
Sanacorp	Ureia	21002312001	1
Sanacorp	Ureia	21002313007	3
Sanacorp	Ureia	21002313016	1
Sanacorp	Ureia	210200201	1
Sanacorp	Ureia	2102002-01	2
Sanacorp	Ureia	21C16-B02-210554	1
Sanacorp	Ureia	21C16-B02-214451	1
sanacorp	Ureia	22002605009	1
Sanacorp	Ureia	22002605009	3
sanacorp	Ureia	2301020-01	1
Sanacorp	Ureia	2301020-01	1
Sanacorp	Ureia	2301020-02	1
Sanacorp	Ureia	62/AKD50s	1
Sanacorp	Ureia	63/AKD1	1
Sanacorp	Ureia	Caelo	1
Sanacorp	Ureia	V016-2019	1
SKW Stickstoffwerke	Ureia	1804007-01	1
SKW	Ureia	1404024-01	1
Spangro 07.02.2014	Ureia	13064226	1
Spangro 17.01.2019	Ureia	18023007	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spangro 22.05.2014	Ureia	13064230	1
Spangro_07.11.2018	Ureia	18023010	1
test	Ureia	test	1
THC/Phönix	Ureia	18023006	1
Träger	Ureia	14107112	1
VDL;05.02.15;10.15EUR	Ureia	14107113	1
WE:Phoenix 11.08.16 …	Ureia	15154111	1

- 229 445 spectra from 1514 *Apo-Ident* customers from a total of 48 659 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ureia* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ureia* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	680	0	152 282
Type B	0	1340	0	200 744
Type C	0	6619	3	229 445

The substance/substance group *Ureia* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1176 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5522 %)
Type C	100.0000 % (> 99.9007 %)	99.9547 % (> 99.9094 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20712	22552	4,52	213,73
21537	22466	3,99	216,32
22315	22466	8,10	211,29
22317	22466	4,94	212,45
22376	22376	0,00	214,08
22466	22466	0,00	215,43
22552	22552	0,00	214,24
23033	23033	0,00	212,27
24294	22466	8,25	211,10
25549	25549	0,00	213,32
26518	26518	0,00	212,53

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Valerato de betametasona**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20026-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Valerato de betametasona; Betamethasoni valeras; Betametosona, valerato

Special notes

When selecting the *Valerato de betametasona* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Valerato de betametasona	10	12	809

Second-stage model

For differentiation of the substance/substance group *Valerato de betametasona* the following second-stage model is used:

- Submodelo 07

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Valerato de betametasona* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fosfato dissódico de prednisolona	80,71	–
⋮	⋮	⋮
Budesonida	>50	34,77
Eritromicina	>50	35,66

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Valerato de betametasona* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Valerato de betametasona*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Valerato de betametasona	13091213	21215	40	20130506
Caelo	Valerato de betametasona	13225507	21588	54	1706018
Euro OTC	Valerato de betametasona	1208014-01	20920	40	20120928
Euro OTC	Valerato de betametasona	1406019-01	21645	60	20140725
Euro OTC	Valerato de betametasona	1510037	22249	60	20151215*
Euro OTC	Valerato de betametasona	1510037	22249SI	30	20151215*
Euro OTC	Valerato de betametasona	1610010	22861	40	20161116*
Euro OTC	Valerato de betametasona	1811008	24349	40	20181207*
Euro OTC	Valerato de betametasona	1811008	24349SI	30	20181207*
Fagron	Valerato de betametasona	12K07-N23	20887	40	20121119
Fagron	Valerato de betametasona	13K29-B32-288243	21566	60	20131210
Fagron	Valerato de betametasona	13K05-B08-292651	21674	60	1511154

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 554 spectra of 12 reference samples from the substance/substance group *Valerato de betametasona*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 408 spectra from a total of 2832 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 881 spectra of 26 reference samples from the substance/substance group *Valerato de betametasona*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Valerato de betametasona	170787	23332	40
Caelo	Valerato de betametasona	172716	23683	40
Caelo	Valerato de betametasona	22001101	26127	38
Caelo	Valerato de betametasona	23002259	26968	40
Euro OTC	Valerato de betametasona	1606023	22716	40
Euro OTC	Valerato de betametasona	1704019	23396	40
Euro OTC	Valerato de betametasona	1801024	23967	40
Euro OTC	Valerato de betametasona	1911001	24982	40
Euro OTC	Valerato de betametasona	2102010	25540	40
Euro OTC	Valerato de betametasona	2202016	26035	40
Euro OTC	Valerato de betametasona	2309023	27009	30
Fagron	Valerato de betametasona	21K09-B05-217898	26171	40
Caelo	Valerato de betametasona	13225507	21588†	6
Caelo	Valerato de betametasona	170787	23332SI	20
Caelo	Valerato de betametasona	172716	23683SI	20
Caelo	Valerato de betametasona	22001101	26127SI	30
Caelo	Valerato de betametasona	23002259	26968SI	34
Euro OTC	Valerato de betametasona	1606023	22716SI	34
Euro OTC	Valerato de betametasona	1610010	22861SI†	30
Euro OTC	Valerato de betametasona	1704019	23396SI	29
Euro OTC	Valerato de betametasona	1801024	23967SI	40
Euro OTC	Valerato de betametasona	1911001	24982SI	40
Euro OTC	Valerato de betametasona	2102010	25540SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Valerato de betametasona	2202016	26035SI	10
Euro OTC	Valerato de betametasona	2309023	27009SI	40
Fagron	Valerato de betametasona	21K09-B05-217898	26171SI	40

- 201 203 spectra from a total of 4031 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5621 spectra from 1248 *Apo-Ident* customers from 861 batches from the substance/substance group *Valerato de betametasona*.

- Among them are spectra of independent samples from 805 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Valerato de betametasona		1
	Valerato de betametasona	1208014-04	1
	Valerato de betametasona	181108-01	1
	Valerato de betametasona	21000036021	3
	Valerato de betametasona	21K09-B05-217891	1
	Valerato de betametasona	21K09-B05-217898	1
	Valerato de betametasona	21K09-B05-22018	1
	Valerato de betametasona	21K09-B05-220180	1
	Valerato de betametasona	21K09-B05-220365	1
	Valerato de betametasona	21k09-B05-222192	1
	Valerato de betametasona	21K09-B05-222192	8
	Valerato de betametasona	21K09-B05-222194	1
	Valerato de betametasona	2200101016	1
	Valerato de betametasona	22001101003	7
	Valerato de betametasona	22001101004	1
	Valerato de betametasona	22001101008	4
	Valerato de betametasona	22001101009	3
	Valerato de betametasona	22001101014	1
	Valerato de betametasona	22001101015	10
	Valerato de betametasona	22001101016	9
	Valerato de betametasona	22001101017	4
	Valerato de betametasona	22001101018	11
	Valerato de betametasona	22001101020	11
	Valerato de betametasona	22001101021	5
	Valerato de betametasona	22001101025	2
	Valerato de betametasona	22001102021	1
	Valerato de betametasona	2202015-51	1
	Valerato de betametasona	2202016-01	10
	Valerato de betametasona	2202016-02	6
	Valerato de betametasona	221101020	1
	Valerato de betametasona	22H25-B07-223527	6
	Valerato de betametasona	22H25-B07-227236	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Valerato de betametasona	22H25-B07-227293	1
	Valerato de betametasona	22HB07223527	1
	Valerato de betametasona	22K07-B08-227496	1
	Valerato de betametasona	22K07B08229283	1
	Valerato de betametasona	22K07-B08-229283	2
	Valerato de betametasona	23003252001	1
	Valerato de betametasona	23003252003	1
	Valerato de betametasona	2309023-01	10
	Valerato de betametasona	B07-2272306	1
	Valerato de betametasona	BV005/1221	1
/Sanacorp	Valerato de betametasona	17078701	1
03110031	Valerato de betametasona	17271603	1
A.H.D.	Valerato de betametasona	13D03-N07	1
Aep	Valerato de betametasona	22001101018	1
AEP	Valerato de betametasona	F02-3737908	1
agron/Krieger	Valerato de betametasona	12B2B-N01	1
AHC 01.07.13 EK 48,05	Valerato de betametasona	12K07-N23	1
AHD 04.10.17 E.k:18,47	Valerato de betametasona	16270514	1
AHD 15.06.16 EK:18,44	Valerato de betametasona	15398505	1
AHD 17.11.14 EK 18,11	Valerato de betametasona	13091205	1
AHD/Euro	Valerato de betametasona	181100801	1
AHD/Fargon	Valerato de betametasona	14H28-Bo1-302865	1
AHD	Valerato de betametasona	1406019-02	2
AHD	Valerato de betametasona	15262607	1
AHD	Valerato de betametasona	15398515	1
AHD	Valerato de betametasona	17078714	1
AHD	Valerato de betametasona	18199902	1
AHD	Valerato de betametasona	22001101015	1
AHDE / Cael 17.02.2015	Valerato de betametasona	13225516	1
AHL	Valerato de betametasona	15398501	1
ALH	Valerato de betametasona	15398512	1
Alliance Haelthcare	Valerato de betametasona	21K09-B05-220180	1
Alliance Health 06.0...	Valerato de betametasona	13091207	1
Alliance healthcare	Valerato de betametasona	13D03-N07	1
Alliance Healthcare	Valerato de betametasona	1610010-01	1
Alliance/EurRho	Valerato de betametasona	1912012-01	1
Alliance	Valerato de betametasona	22001101017	1
alliance	Valerato de betametasona	2202016-01	1
Allianz Healthcare 2...	Valerato de betametasona	15075802	1
Anzag	Valerato de betametasona	12L11-N01	1
Anzag	Valerato de betametasona	1819908	1
Anzag	Valerato de betametasona	21000036003	2
Audor Pharma	Valerato de betametasona	APBV010/0516B	5
Biomed / Gehe	Valerato de betametasona	1510037-01	1
Bombastus	Valerato de betametasona	12L11-N01	1
Bombastus	Valerato de betametasona	1510037-01	1
Bombastus	Valerato de betametasona	1704019-01	4
Bombatus	Valerato de betametasona	1801024-01	3
Cael Sanacorp 05.02.2016	Valerato de betametasona	14H28-B01-302864	1
Caello/Sanacorp	Valerato de betametasona	15075803	1
Caelo	Valerato de betametasona		3
Caelo	Valerato de betametasona	10296701	1
Caelo	Valerato de betametasona	10296705	2
Caelo	Valerato de betametasona	10296707	1
Caelo	Valerato de betametasona	1108045-03	4
Caelo	Valerato de betametasona	1113	1
Caelo	Valerato de betametasona	11131905	1
Caelo	Valerato de betametasona	11131909	1
Caelo	Valerato de betametasona	11131914	1
Caelo	Valerato de betametasona	11131917	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de betametasona	1131914	1
Caelo	Valerato de betametasona	1199932	1
Caelo	Valerato de betametasona	12003402	1
Caelo	Valerato de betametasona	12003403	7
Caelo	Valerato de betametasona	12003404	1
Caelo	Valerato de betametasona	12003405	8
Caelo	Valerato de betametasona	12003406	6
Caelo	Valerato de betametasona	12003407	1
Caelo	Valerato de betametasona	12003409	1
Caelo	Valerato de betametasona	12003410	1
Caelo	Valerato de betametasona	12003411	3
Caelo	Valerato de betametasona	1208014-01	1
Caelo	Valerato de betametasona	1208014-03	1
Caelo	Valerato de betametasona	12207004	1
Caelo	Valerato de betametasona	12229802	3
Caelo	Valerato de betametasona	12229804	4
Caelo	Valerato de betametasona	12229805	9
Caelo	Valerato de betametasona	12229806	6
Caelo	Valerato de betametasona	12229808	12
Caelo	Valerato de betametasona	12229809	2
Caelo	Valerato de betametasona	12229810	4
Caelo	Valerato de betametasona	12229811	7
Caelo	Valerato de betametasona	12229812	9
Caelo	Valerato de betametasona	12229813	2
Caelo	Valerato de betametasona	123345	1
Caelo	Valerato de betametasona	129711-5471	1
Caelo	Valerato de betametasona	12B28-N01	1
Caelo	Valerato de betametasona	12g09-n07	1
Caelo	Valerato de betametasona	12G09-N07	3
Caelo	Valerato de betametasona	12K07-N23	1
Caelo	Valerato de betametasona	12L11-N01	1
Caelo	Valerato de betametasona	13012015C	1
Caelo	Valerato de betametasona	13091201	2
Caelo	Valerato de betametasona	13091203	12
Caelo	Valerato de betametasona	13091204	4
Caelo	Valerato de betametasona	13091205	11
Caelo	Valerato de betametasona	13091206	1
Caelo	Valerato de betametasona	13091207	8
Caelo	Valerato de betametasona	13091209	4
Caelo	Valerato de betametasona	13091210	3
Caelo	Valerato de betametasona	13091211	3
Caelo	Valerato de betametasona	13091212	6
Caelo	Valerato de betametasona	13091213	6
Caelo	Valerato de betametasona	13225502	2
Caelo	Valerato de betametasona	13225503	9
Caelo	Valerato de betametasona	13225504	9
Caelo	Valerato de betametasona	13225505	12
Caelo	Valerato de betametasona	13225507	2
Caelo	Valerato de betametasona	13225508	9
Caelo	Valerato de betametasona	13225509	2
Caelo	Valerato de betametasona	13225515	9
Caelo	Valerato de betametasona	13225516	10
Caelo	Valerato de betametasona	13225607	1
Caelo	Valerato de betametasona	13923	1
Caelo	Valerato de betametasona	13D03-N07	3
Caelo	Valerato de betametasona	13G19-N01	1
Caelo	Valerato de betametasona	13K05_B08_292652	1
Caelo	Valerato de betametasona	13K29-B32-288247	1
Caelo	Valerato de betametasona	14031407	1
Caelo	Valerato de betametasona	1406019-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de betametasona	1406019-02	3
Caelo	Valerato de betametasona	140601903	1
Caelo	Valerato de betametasona	1406019-03	4
Caelo	Valerato de betametasona	14188602	2
Caelo	Valerato de betametasona	14188603	5
Caelo	Valerato de betametasona	14188604	8
Caelo	Valerato de betametasona	14188605	1
Caelo	Valerato de betametasona	14188606	1
Caelo	Valerato de betametasona	14188608	8
Caelo	Valerato de betametasona	14188609	5
Caelo	Valerato de betametasona	14188610	7
Caelo	Valerato de betametasona	14188617	3
Caelo	Valerato de betametasona	14188619	3
Caelo	Valerato de betametasona	1488609	1
Caelo	Valerato de betametasona	1488610	1
Caelo	Valerato de betametasona	14C19-B02-292653	1
Caelo	Valerato de betametasona	14G30-B05	1
Caelo	Valerato de betametasona	14G30-B05-309520	1
Caelo	Valerato de betametasona	14H28-B01-302865	1
Caelo	Valerato de betametasona	15/16-B07-317416	1
Caelo	Valerato de betametasona	15/16-B07-317417	1
Caelo	Valerato de betametasona	15/16-B07-319228	2
Caelo	Valerato de betametasona	15075802	22
Caelo	Valerato de betametasona	150758022	1
Caelo	Valerato de betametasona	15075803	9
Caelo	Valerato de betametasona	150758036	1
Caelo	Valerato de betametasona	15075804	8
Caelo	Valerato de betametasona	15075805	8
Caelo	Valerato de betametasona	15075809	4
Caelo	Valerato de betametasona	15075810	9
Caelo	Valerato de betametasona	15075811	1
Caelo	Valerato de betametasona	15075812	3
Caelo	Valerato de betametasona	1510037-01	2
Caelo	Valerato de betametasona	1516-B07-319228	1
Caelo	Valerato de betametasona	1526213	1
Caelo	Valerato de betametasona	15262602	8
Caelo	Valerato de betametasona	15262603	15
Caelo	Valerato de betametasona	15262604	14
Caelo	Valerato de betametasona	15262606	4
Caelo	Valerato de betametasona	15262607	7
Caelo	Valerato de betametasona	15262609	3
Caelo	Valerato de betametasona	15262610	4
Caelo	Valerato de betametasona	15262612	1
Caelo	Valerato de betametasona	15262613	1
Caelo	Valerato de betametasona	1526604	1
Caelo	Valerato de betametasona	1538506	1
Caelo	Valerato de betametasona	15395512	1
Caelo	Valerato de betametasona	15398501	23
Caelo	Valerato de betametasona	15398502	1
Caelo	Valerato de betametasona	15398503	2
Caelo	Valerato de betametasona	15398504	3
Caelo	Valerato de betametasona	15398505	17
Caelo	Valerato de betametasona	15398506	30
Caelo	Valerato de betametasona	15398512	22
Caelo	Valerato de betametasona	15398513	4
Caelo	Valerato de betametasona	15398514	3
Caelo	Valerato de betametasona	15398515	27
Caelo	Valerato de betametasona	15B24-B04	1
Caelo	Valerato de betametasona	15B24-B04-307016	1
Caelo	Valerato de betametasona	15F16-B04-314054	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de betametasona	15F16-B04-315327	1
Caelo	Valerato de betametasona	15L21-B03-318663	1
Caelo	Valerato de betametasona	160216BV	1
Caelo	Valerato de betametasona	160501	1
Caelo	Valerato de betametasona	160503	1
Caelo	Valerato de betametasona	1606023-01	4
Caelo	Valerato de betametasona	1610010-01	5
Caelo	Valerato de betametasona	161125BV/15398512	1
Caelo	Valerato de betametasona	16270501	17
Caelo	Valerato de betametasona	16270502	37
Caelo	Valerato de betametasona	16270503	18
Caelo	Valerato de betametasona	16270504	1
Caelo	Valerato de betametasona	16270505	16
Caelo	Valerato de betametasona	16270508	2
Caelo	Valerato de betametasona	16270509	9
Caelo	Valerato de betametasona	1627051	1
Caelo	Valerato de betametasona	16270511	26
Caelo	Valerato de betametasona	16270513	22
Caelo	Valerato de betametasona	16270514	9
Caelo	Valerato de betametasona	16720513	1
Caelo	Valerato de betametasona	16B18-B02-320971	2
Caelo	Valerato de betametasona	16B18-B02-322121	2
Caelo	Valerato de betametasona	16B18-B02-324798	1
Caelo	Valerato de betametasona	16E23-B03	1
Caelo	Valerato de betametasona	16E23-B03-324799	2
Caelo	Valerato de betametasona	16E23-B03-324800	1
Caelo	Valerato de betametasona	16e23-b03-328128	1
Caelo	Valerato de betametasona	16E23-B03-328128	3
Caelo	Valerato de betametasona	16H22-B06-331273	1
Caelo	Valerato de betametasona	16H22B06332351	1
Caelo	Valerato de betametasona	16H22-B06-332351	1
Caelo	Valerato de betametasona	17/251/Bv	1
Caelo	Valerato de betametasona	170401901	4
Caelo	Valerato de betametasona	1704019-01	18
Caelo	Valerato de betametasona	17078103	1
Caelo	Valerato de betametasona	1707814	1
Caelo	Valerato de betametasona	1707815	2
Caelo	Valerato de betametasona	1707819	1
Caelo	Valerato de betametasona	17078701	25
Caelo	Valerato de betametasona	17078702	1
Caelo	Valerato de betametasona	17078703	35
Caelo	Valerato de betametasona	17078704	7
Caelo	Valerato de betametasona	17078705	1
Caelo	Valerato de betametasona	17078707	1
Caelo	Valerato de betametasona	17078711	7
Caelo	Valerato de betametasona	17078712	13
Caelo	Valerato de betametasona	17078713	19
Caelo	Valerato de betametasona	17078714	17
Caelo	Valerato de betametasona	17078715	16
Caelo	Valerato de betametasona	17078716	1
Caelo	Valerato de betametasona	17078719	18
Caelo	Valerato de betametasona	17078720	25
Caelo	Valerato de betametasona	1708701	1
Caelo	Valerato de betametasona	17196001	1
Caelo	Valerato de betametasona	17271601	7
Caelo	Valerato de betametasona	17271602	1
Caelo	Valerato de betametasona	17271603	29
Caelo	Valerato de betametasona	17271604	9
Caelo	Valerato de betametasona	1729002	1
Caelo	Valerato de betametasona	17329001	29

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de betametasona	17329002	39
Caelo	Valerato de betametasona	17329003	17
Caelo	Valerato de betametasona	17329004	6
Caelo	Valerato de betametasona	17329008	10
Caelo	Valerato de betametasona	17329011	7
Caelo	Valerato de betametasona	17329015	15
Caelo	Valerato de betametasona	17329017	10
Caelo	Valerato de betametasona	17329018	76
Caelo	Valerato de betametasona	1732901803110025	1
Caelo	Valerato de betametasona	17329019	4
Caelo	Valerato de betametasona	173296011	1
Caelo	Valerato de betametasona	1739002	3
Caelo	Valerato de betametasona	17C29-B04	2
Caelo	Valerato de betametasona	17C29-B04-334329	1
Caelo	Valerato de betametasona	17C29-B04-335676	2
Caelo	Valerato de betametasona	17G31B04338575	1
Caelo	Valerato de betametasona	17G31-B04-338575	1
Caelo	Valerato de betametasona	17G31-B04-341576	1
Caelo	Valerato de betametasona	17K16-B0/8-347310	1
Caelo	Valerato de betametasona	17K16-B08	1
Caelo	Valerato de betametasona	17K16-B08-345541	3
Caelo	Valerato de betametasona	17K16-B08-347309	2
Caelo	Valerato de betametasona	17K16-B08-347912	1
Caelo	Valerato de betametasona	1801024-01	12
Caelo	Valerato de betametasona	18071403	1
Caelo	Valerato de betametasona	1811008	1
Caelo	Valerato de betametasona	181100801	1
Caelo	Valerato de betametasona	1811008-01	3
Caelo	Valerato de betametasona	18121206	1
Caelo	Valerato de betametasona	18189907	1
Caelo	Valerato de betametasona	1819908	1
Caelo	Valerato de betametasona	1819918	3
Caelo	Valerato de betametasona	1819924	1
Caelo	Valerato de betametasona	1819932	1
Caelo	Valerato de betametasona	181999007	1
Caelo	Valerato de betametasona	18199902	43
Caelo	Valerato de betametasona	18199903	2
Caelo	Valerato de betametasona	18199906	10
Caelo	Valerato de betametasona	18199907	37
Caelo	Valerato de betametasona	1819990705/2023	1
Caelo	Valerato de betametasona	18199908	15
Caelo	Valerato de betametasona	18199914	4
Caelo	Valerato de betametasona	18199915	4
Caelo	Valerato de betametasona	18199916	19
Caelo	Valerato de betametasona	18199918	50
Caelo	Valerato de betametasona	18199923P-200116-2	1
Caelo	Valerato de betametasona	18199924	19
Caelo	Valerato de betametasona	18199926	4
Caelo	Valerato de betametasona	18199930	8
Caelo	Valerato de betametasona	18199932	46
Caelo	Valerato de betametasona	18199933	36
Caelo	Valerato de betametasona	18199937	2
Caelo	Valerato de betametasona	18199938	8
Caelo	Valerato de betametasona	18G03-B03-351731	1
Caelo	Valerato de betametasona	18I27-B05-354880	1
Caelo	Valerato de betametasona	1912012-01	2
Caelo	Valerato de betametasona	19220009	1
Caelo	Valerato de betametasona	1922070003	1
Caelo	Valerato de betametasona	192207001	18
Caelo	Valerato de betametasona	192207002	42

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de betametasona	192207003	32
Caelo	Valerato de betametasona	192207004	4
Caelo	Valerato de betametasona	192207006	11
Caelo	Valerato de betametasona	192207009	27
Caelo	Valerato de betametasona	192207010	20
Caelo	Valerato de betametasona	192207012	21
Caelo	Valerato de betametasona	19220702	34
Caelo	Valerato de betametasona	19220703	7
Caelo	Valerato de betametasona	19220704	26
Caelo	Valerato de betametasona	19220705	42
Caelo	Valerato de betametasona	19220706	1
Caelo	Valerato de betametasona	19220707012	1
Caelo	Valerato de betametasona	19g30-b02-363673	1
Caelo	Valerato de betametasona	19g30-b02-363693	1
Caelo	Valerato de betametasona	20002685001	6
Caelo	Valerato de betametasona	20B18-F07-370009	2
Caelo	Valerato de betametasona	20B18-F07-370010	1
Caelo	Valerato de betametasona	21000026003	2
Caelo	Valerato de betametasona	210000360010	2
Caelo	Valerato de betametasona	21000036003	58
Caelo	Valerato de betametasona	21000036004	22
Caelo	Valerato de betametasona	210000360063	1
Caelo	Valerato de betametasona	21000036007	2
Caelo	Valerato de betametasona	21000036008	11
Caelo	Valerato de betametasona	21000036010	32
Caelo	Valerato de betametasona	21000036011	1
Caelo	Valerato de betametasona	21000036013	1
Caelo	Valerato de betametasona	21000036016	19
Caelo	Valerato de betametasona	21000036017	39
Caelo	Valerato de betametasona	21000036018	2
Caelo	Valerato de betametasona	21000036019	1
Caelo	Valerato de betametasona	21000036020	19
Caelo	Valerato de betametasona	21000036021	19
Caelo	Valerato de betametasona	21000036022	2
Caelo	Valerato de betametasona	2100003610	1
Caelo	Valerato de betametasona	2100036003	4
Caelo	Valerato de betametasona	2100036004	1
Caelo	Valerato de betametasona	2100036010	2
Caelo	Valerato de betametasona	2100036016	1
Caelo	Valerato de betametasona	2100036020	1
Caelo	Valerato de betametasona	2100036021	1
Caelo	Valerato de betametasona	210003610	1
Caelo	Valerato de betametasona	210112	1
Caelo	Valerato de betametasona	210201001	1
Caelo	Valerato de betametasona	2102010-02	1
Caelo	Valerato de betametasona	21G28-B02-213516	1
Caelo	Valerato de betametasona	22001101002	2
Caelo	Valerato de betametasona	22001101003	1
Caelo	Valerato de betametasona	22001101004	3
Caelo	Valerato de betametasona	22001101005	16
Caelo	Valerato de betametasona	22001101009	5
Caelo	Valerato de betametasona	22001101015	2
Caelo	Valerato de betametasona	22001101016	2
Caelo	Valerato de betametasona	22001101018	1
Caelo	Valerato de betametasona	2x12229813	1
Caelo	Valerato de betametasona	31(17329018)	1
Caelo	Valerato de betametasona	311002517078712	1
Caelo	Valerato de betametasona	3303	1
Caelo	Valerato de betametasona	534210000363	1
Caelo	Valerato de betametasona	8081502	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de betametasona	922070101	1
Caelo	Valerato de betametasona	APPV010/0516B	1
Caelo	Valerato de betametasona	B03041205	1
Caelo	Valerato de betametasona	BV018/0715	2
Caelo	Valerato de betametasona	BV109/0519	1
Caelo	Valerato de betametasona	BV-BLT225/0514	1
Caelo	Valerato de betametasona	F07-3667709	1
Caelo	Valerato de betametasona	NT0597M	1
Caeolo /Sana	Valerato de betametasona	18199903	1
Caesar & Lorenz GmbH	Valerato de betametasona	15075805	1
Caesar & Lorenz GmbH	Valerato de betametasona	16270501	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036020	1
Caesar & Loretz GmbH…	Valerato de betametasona	19220702	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036004	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199938	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101005	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036011	1
Caesar & Loretz GmbH…	Valerato de betametasona	120801402	1
Caesar & Loretz GmbH…	Valerato de betametasona	10296707	1
Caesar & Loretz GmbH…	Valerato de betametasona	12003404	1
Caesar & Loretz GmbH…	Valerato de betametasona	12003409	2
Caesar & Loretz GmbH…	Valerato de betametasona	12229809	1
Caesar & Loretz GmbH…	Valerato de betametasona	13091206	2
Caesar & Loretz GmbH…	Valerato de betametasona	13091211	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036008	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101005	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199915	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101015	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199916	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101009	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101005	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199902	1
Caesar & Loretz GmbH/	Valerato de betametasona	17329018	1
Caesar & Loretz GmbH/AEP	Valerato de betametasona	18199924	1
Caesar & Loretz GmbH/E	Valerato de betametasona	18199938	1
Caesar & Loretz GmbH/E	Valerato de betametasona	21000036016	1
Caesar & Loretz GmbH…	Valerato de betametasona	20002685001	2
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	18199903	1
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	18199908	1
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	18199916	1
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	19220702	1
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	21000036010	1
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	21000036016	1
Caesar & Loretz GmbH/Gehe	Valerato de betametasona	22001101021	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036010	1
Caesar & Loretz GmbH/Gö	Valerato de betametasona	21000036021	2
Caesar & Loretz GmbH…	Valerato de betametasona	18199918	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036003	3
Caesar & Loretz GmbH…	Valerato de betametasona	192207010	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199918	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199933	1
Caesar & Loretz GmbH…	Valerato de betametasona	192207010	1
Caesar & Loretz GmbH…	Valerato de betametasona	19220705	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036016	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101004	1
Caesar & Loretz GmbH…	Valerato de betametasona	22001101015	1
Caesar & Loretz GmbH/K	Valerato de betametasona	19220702	1
Caesar & Loretz GmbH/Kehr	Valerato de betametasona	21000036021	1
Caesar & Loretz GmbH…	Valerato de betametasona	18199918	1
Caesar & Loretz GmbH…	Valerato de betametasona	21000036010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Valerato de betametasona	18199907	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199908	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199918	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199933	1
Caesar & Loretz GmbH...	Valerato de betametasona	192207002	1
Caesar & Loretz GmbH...	Valerato de betametasona	192207010	2
Caesar & Loretz GmbH...	Valerato de betametasona	21000036003	3
Caesar & Loretz GmbH...	Valerato de betametasona	21000036010	1
Caesar & Loretz GmbH...	Valerato de betametasona	21000036021	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199915	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199924	2
Caesar & Loretz GmbH...	Valerato de betametasona	18G03-B03-352460	1
Caesar & Loretz GmbH...	Valerato de betametasona	19220704	2
Caesar & Loretz GmbH...	Valerato de betametasona	20002685001	1
Caesar & Loretz GmbH...	Valerato de betametasona	21000036003	2
Caesar & Loretz GmbH...	Valerato de betametasona	21000036004	1
Caesar & Loretz GmbH...	Valerato de betametasona	BV116/0819	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199918	1
Caesar & Loretz GmbH...	Valerato de betametasona	21000036017	2
Caesar & Loretz GmbH...	Valerato de betametasona	192207002	1
Caesar & Loretz GmbH...	Valerato de betametasona	192207009	3
Caesar & Loretz GmbH...	Valerato de betametasona	192207010	2
Caesar & Loretz GmbH...	Valerato de betametasona	19220705	1
Caesar & Loretz GmbH...	Valerato de betametasona	21000036003	2
Caesar & Loretz GmbH...	Valerato de betametasona	22001101005	1
Caesar & Loretz GmbH...	Valerato de betametasona	22001101015	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199915	1
Caesar & Loretz GmbH...	Valerato de betametasona	18199932	2
Caesar & Loretz GmbH...	Valerato de betametasona	19220702	1
Caesar & Loretz GmbH...	Valerato de betametasona	19220703	1
Caesar & Loretz GmbH...	Valerato de betametasona	21000036004	2
Caesar & Loretz GmbH...	Valerato de betametasona	21000036017	1
Caesar & Loretz GmbH	Valerato de betametasona	13225504	1
Caesar & Loretz GmbH	Valerato de betametasona	16270511	1
Caesar & Loretz GmbH	Valerato de betametasona	17078701	1
Caesar & Loretz GmbH	Valerato de betametasona	17329001	1
Caesar & Loretz GmbH	Valerato de betametasona	17329002	1
Caesar & Loretz GmbH	Valerato de betametasona	17329004	1
Caesar & Loretz GmbH	Valerato de betametasona	17329015	1
Caesar & Loretz GmbH	Valerato de betametasona	17329018	5
Caesar & Loretz GmbH	Valerato de betametasona	17K16B08345555	1
Caesar & Loretz GmbH	Valerato de betametasona	1811008-01	2
Caesar & Loretz GmbH	Valerato de betametasona	1819930	1
Caesar & Loretz GmbH	Valerato de betametasona	18199902	1
Caesar & Loretz GmbH	Valerato de betametasona	18199903	1
Caesar & Loretz GmbH	Valerato de betametasona	18199906	1
Caesar & Loretz GmbH	Valerato de betametasona	18199907	8
Caesar & Loretz GmbH	Valerato de betametasona	18199908	3
Caesar & Loretz GmbH	Valerato de betametasona	18199914	1
Caesar & Loretz GmbH	Valerato de betametasona	18199915	4
Caesar & Loretz GmbH	Valerato de betametasona	18199916	5
Caesar & Loretz GmbH	Valerato de betametasona	18199918	15
Caesar & Loretz GmbH	Valerato de betametasona	18199923	1
Caesar & Loretz GmbH	Valerato de betametasona	18199924	6
Caesar & Loretz GmbH	Valerato de betametasona	18199930	1
Caesar & Loretz GmbH	Valerato de betametasona	18199932	7
Caesar & Loretz GmbH	Valerato de betametasona	18199933	11
Caesar & Loretz GmbH	Valerato de betametasona	18199937	1
Caesar & Loretz GmbH	Valerato de betametasona	18199938	5
Caesar & Loretz GmbH	Valerato de betametasona	18G03-B03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Valerato de betametasona	192207001	8
Caesar & Loretz GmbH	Valerato de betametasona	192207002	12
Caesar & Loretz GmbH	Valerato de betametasona	192207003	8
Caesar & Loretz GmbH	Valerato de betametasona	192207004	1
Caesar & Loretz GmbH	Valerato de betametasona	192207005	1
Caesar & Loretz GmbH	Valerato de betametasona	192207006	1
Caesar & Loretz GmbH	Valerato de betametasona	192207009	5
Caesar & Loretz GmbH	Valerato de betametasona	192207010	5
Caesar & Loretz GmbH	Valerato de betametasona	192207012	11
Caesar & Loretz GmbH	Valerato de betametasona	19220702	12
Caesar & Loretz GmbH	Valerato de betametasona	19220703	1
Caesar & Loretz GmbH	Valerato de betametasona	19220704	11
Caesar & Loretz GmbH	Valerato de betametasona	19220705	3
Caesar & Loretz GmbH	Valerato de betametasona	19220706	1
Caesar & Loretz GmbH	Valerato de betametasona	19220707	1
Caesar & Loretz GmbH	Valerato de betametasona	1922207002	1
Caesar & Loretz GmbH	Valerato de betametasona	21000036001	1
Caesar & Loretz GmbH	Valerato de betametasona	21000036003	16
Caesar & Loretz GmbH	Valerato de betametasona	21000036004	13
Caesar & Loretz GmbH	Valerato de betametasona	21000036007	2
Caesar & Loretz GmbH	Valerato de betametasona	21000036008	6
Caesar & Loretz GmbH	Valerato de betametasona	21000036010	8
Caesar & Loretz GmbH	Valerato de betametasona	21000036011	1
Caesar & Loretz GmbH	Valerato de betametasona	21000036015	1
Caesar & Loretz GmbH	Valerato de betametasona	21000036016	12
Caesar & Loretz GmbH	Valerato de betametasona	21000036017	13
Caesar & Loretz GmbH	Valerato de betametasona	21000036018	1
Caesar & Loretz GmbH	Valerato de betametasona	21000036019	3
Caesar & Loretz GmbH	Valerato de betametasona	21000036020	8
Caesar & Loretz GmbH	Valerato de betametasona	21000036021	7
Caesar & Loretz GmbH	Valerato de betametasona	21000036023	1
Caesar & Loretz GmbH	Valerato de betametasona	22001101002	1
Caesar & Loretz GmbH	Valerato de betametasona	22001101004	2
Caesar & Loretz GmbH	Valerato de betametasona	22001101005	2
Caesar & Loretz GmbH	Valerato de betametasona	22001101009	3
Caesar & Loretz GmbH	Valerato de betametasona	22001101015	2
Caesar & Loretz GmbH	Valerato de betametasona	22001101016	1
Caesar & Loretz GmbH	Valerato de betametasona	22001101023	2
Caesar & Loretz/Gehe	Valerato de betametasona	18199932	1
Caesar & Loretz/Geil...	Valerato de betametasona	192207001	1
Caesar & Loretz	Valerato de betametasona	17329016	1
Caesar & Loretz	Valerato de betametasona	21000036008	1
Caesar &Loretz GmbH	Valerato de betametasona	11131917	1
Caesar Loretz	Valerato de betametasona	192207010	1
Caesar und Loretz	Valerato de betametasona	15075803	1
Caesar&Lorenz	Valerato de betametasona	21000036016	1
Caesar&Loretz GmbH,P...	Valerato de betametasona	16270509	1
Caesar&Loretz GmbH/Anzag	Valerato de betametasona	15075802	1
Caesar&Loretz GmbH	Valerato de betametasona	15262609	1
caesar&loretz,phönix	Valerato de betametasona	14188606	1
Caesar/Lorenz	Valerato de betametasona	12003403	1
Caleo/Phönix	Valerato de betametasona	1522609	1
Carlo/Gehe	Valerato de betametasona	19220702	1
Carlo/Phönix/46,64	Valerato de betametasona	18199924	1
Cealo/Gehe	Valerato de betametasona	17329002	1
Cealo/Gehe	Valerato de betametasona	1739002	1
Cealo/Gehe	Valerato de betametasona	1801024-01	1
Cealo/Noweda	Valerato de betametasona	16270509	2
Cealo	Valerato de betametasona	17078716	1
Crystal PH/Oberlinde...	Valerato de betametasona	C0073/114040	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Dr. Aug. Wolff GmbH ...	Valerato de betametasona	192207012	1
E Plus	Valerato de betametasona	16270502	1
E Plus	Valerato de betametasona	17329002	1
Ebert & Jacobi	Valerato de betametasona	14188606	1
Ebert & Jacobi	Valerato de betametasona	15075810	1
Ebert u. Jacobi 1...	Valerato de betametasona	15/16-B07-317417	1
Eigenherstellung	Valerato de betametasona	9070313	1
EuRho / Phoenix	Valerato de betametasona	1704019-01	1
EuRho /Gumo	Valerato de betametasona	1911001-01	1
EuRho/Noweda 02.06.2022	Valerato de betametasona	2102010	1
EuRho/Noweda 11.11.2020	Valerato de betametasona	1912012-01	1
EuRho/Noweda	Valerato de betametasona	1911001-01	16
EuRho/Phönix	Valerato de betametasona	2102010-01	1
EuRho/Sanacorp	Valerato de betametasona	1911001-01	1
EuRho/Spangro	Valerato de betametasona	1811008-01	2
EuRho	Valerato de betametasona	1208014-01	2
EuRho	Valerato de betametasona	1208014-02	1
EuRho	Valerato de betametasona	1610010-01	2
Eurho	Valerato de betametasona	1801024-01	1
EuRho	Valerato de betametasona	180102401	1
EuRho	Valerato de betametasona	1801024-01	4
EuRho	Valerato de betametasona	181008-01	1
Eurho	Valerato de betametasona	1811008-01	1
Eurho	Valerato de betametasona	1911001-01	1
EuRho	Valerato de betametasona	1911001-01	1
EuRho	Valerato de betametasona	1911001-02	1
EuRho	Valerato de betametasona	1912012-01	1
EuRho	Valerato de betametasona	2102010-01	2
Euro / Gehe	Valerato de betametasona	1912012-12	1
Euro OTC	Valerato de betametasona		1
Euro OTC	Valerato de betametasona	1031707	1
Euro OTC	Valerato de betametasona	110804-02	1
Euro OTC	Valerato de betametasona	1108045-01	2
Euro OTC	Valerato de betametasona	1108045-02	3
Euro OTC	Valerato de betametasona	110804503	1
Euro OTC	Valerato de betametasona	1108045-03	7
Euro OTC	Valerato de betametasona	1206014-02	1
Euro OTC	Valerato de betametasona	1208014-01	12
Euro OTC	Valerato de betametasona	120801402	2
Euro OTC	Valerato de betametasona	1208014-02	12
Euro OTC	Valerato de betametasona	120801403	1
Euro OTC	Valerato de betametasona	1208014-03	4
Euro OTC	Valerato de betametasona	120801404	1
Euro OTC	Valerato de betametasona	1208014-04	4
Euro OTC	Valerato de betametasona	120812-02	1
Euro OTC	Valerato de betametasona	12L11-N01	1
Euro OTC	Valerato de betametasona	1311039	1
Euro OTC	Valerato de betametasona	131103901	1
Euro OTC	Valerato de betametasona	1311039-01	22
Euro OTC	Valerato de betametasona	131139-01	1
Euro OTC	Valerato de betametasona	13D03-N07	1
Euro OTC	Valerato de betametasona	13K29-B32-289364	1
Euro OTC	Valerato de betametasona	1406011903	1
Euro OTC	Valerato de betametasona	140601901	1
Euro OTC	Valerato de betametasona	1406019-01	25
Euro OTC	Valerato de betametasona	140601902	1
Euro OTC	Valerato de betametasona	1406019-02	23
Euro OTC	Valerato de betametasona	140601903	2
Euro OTC	Valerato de betametasona	1406019-03	32
Euro OTC	Valerato de betametasona	14C19-B02-292650	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Valerato de betametasona	15/16-B07-319228	1
Euro OTC	Valerato de betametasona	1510037	1
Euro OTC	Valerato de betametasona	151003701	1
Euro OTC	Valerato de betametasona	1510037-01	24
Euro OTC	Valerato de betametasona	1510037-07	1
Euro OTC	Valerato de betametasona	1516B07317416	1
Euro OTC	Valerato de betametasona	15398501	1
Euro OTC	Valerato de betametasona	15F16/B04-314054	1
Euro OTC	Valerato de betametasona	1606023-01	41
Euro OTC	Valerato de betametasona	160623-01	1
Euro OTC	Valerato de betametasona	16100100-01	1
Euro OTC	Valerato de betametasona	161001001	1
Euro OTC	Valerato de betametasona	1610010-01	55
Euro OTC	Valerato de betametasona	1610010-03	1
Euro OTC	Valerato de betametasona	16270505	1
Euro OTC	Valerato de betametasona	16E23-B03-328128	3
Euro OTC	Valerato de betametasona	1704018-01	1
Euro OTC	Valerato de betametasona	1704019	2
Euro OTC	Valerato de betametasona	1704019_01	1
Euro OTC	Valerato de betametasona	1704019-0	1
Euro OTC	Valerato de betametasona	170401901	5
Euro OTC	Valerato de betametasona	1704019-01	140
Euro OTC	Valerato de betametasona	1704019-1	1
Euro OTC	Valerato de betametasona	1704021-04	1
Euro OTC	Valerato de betametasona	170419-01	1
Euro OTC	Valerato de betametasona	17078701	1
Euro OTC	Valerato de betametasona	17078703	1
Euro OTC	Valerato de betametasona	17078720	1
Euro OTC	Valerato de betametasona	17271603	3
Euro OTC	Valerato de betametasona	17329001	1
Euro OTC	Valerato de betametasona	1739002	1
Euro OTC	Valerato de betametasona	1740419-01	1
Euro OTC	Valerato de betametasona	17C29-B04-336434	1
Euro OTC	Valerato de betametasona	17K16-B08-345541	1
Euro OTC	Valerato de betametasona	17o4019-01	1
Euro OTC	Valerato de betametasona	18010024-01	1
Euro OTC	Valerato de betametasona	1801024	1
Euro OTC	Valerato de betametasona	1801024_01	1
Euro OTC	Valerato de betametasona	180102401	2
Euro OTC	Valerato de betametasona	1801024-01	133
Euro OTC	Valerato de betametasona	180104-01	1
Euro OTC	Valerato de betametasona	181008-01	1
Euro OTC	Valerato de betametasona	1811008	1
Euro OTC	Valerato de betametasona	181100801	5
Euro OTC	Valerato de betametasona	1811008-01	124
Euro OTC	Valerato de betametasona	1811008-1	2
Euro OTC	Valerato de betametasona	1811024-01	1
Euro OTC	Valerato de betametasona	18199902	1
Euro OTC	Valerato de betametasona	18199907	1
Euro OTC	Valerato de betametasona	190451504	1
Euro OTC	Valerato de betametasona	191001-01	2
Euro OTC	Valerato de betametasona	191100101	1
Euro OTC	Valerato de betametasona	1911001-01	132
Euro OTC	Valerato de betametasona	1911001-02	6
Euro OTC	Valerato de betametasona	191101-01	1
Euro OTC	Valerato de betametasona	1911011-01	1
Euro OTC	Valerato de betametasona	1912012-01	20
Euro OTC	Valerato de betametasona	2014Q1181	1
Euro OTC	Valerato de betametasona	20906	1
Euro OTC	Valerato de betametasona	2102010	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Valerato de betametasona	210201001	2
Euro OTC	Valerato de betametasona	2102010-01	65
Euro OTC	Valerato de betametasona	2102010-02	21
Euro OTC	Valerato de betametasona	210210-01	1
Euro OTC	Valerato de betametasona	2202016-01	24
Euro OTC	Valerato de betametasona	2507211181	1
Euro OTC	Valerato de betametasona	29061805	1
Euro OTC	Valerato de betametasona	3313U-01181	1
Euro OTC	Valerato de betametasona	7071802	1
Euro OTC	Valerato de betametasona	BV116/1117	1
Euro OTC	Valerato de betametasona	BV-BLT221/0314	1
Euro Pharma/Noweda	Valerato de betametasona	1912012-01	6
euro//Noweda	Valerato de betametasona	1801024-01	2
Euro/Alliance Healthcare	Valerato de betametasona	1510037-01	1
Euro/direkt	Valerato de betametasona	1704019-01	1
Euro/Gehe	Valerato de betametasona	1704019-01	1
Euro/Sanacorp	Valerato de betametasona	1801024-01	2
Euro	Valerato de betametasona	1406019-03	3
Euro	Valerato de betametasona	1801024-01	2
Euroo	Valerato de betametasona	1406019-03	1
Europ Ots Pharma	Valerato de betametasona	12111-NO1	1
EurRho/Gehe	Valerato de betametasona	1610010-01	1
Fagon / Noweda	Valerato de betametasona	21G-28-B02-213663	1
Fagon/Noweda	Valerato de betametasona	F07-3667806	1
Fagron	Valerato de betametasona		3
Fagron	Valerato de betametasona	1018E-01181	1
Fagron	Valerato de betametasona	11A04-N02	1
Fagron	Valerato de betametasona	11E18-N03	3
Fagron	Valerato de betametasona	11K18-N09	2
Fagron	Valerato de betametasona	11K-18-N09	1
Fagron	Valerato de betametasona	120801402	1
Fagron	Valerato de betametasona	123649978B	1
Fagron	Valerato de betametasona	12B28-N01	8
Fagron	Valerato de betametasona	12G09-N07	23
Fagron	Valerato de betametasona	12K07N23	1
Fagron	Valerato de betametasona	12K07-N23	6
Fagron	Valerato de betametasona	12L11-N01	18
Fagron	Valerato de betametasona	12L11-NO1	1
Fagron	Valerato de betametasona	13/17-B08-292649	2
Fagron	Valerato de betametasona	1311039-01	1
Fagron	Valerato de betametasona	13d03-n07	3
Fagron	Valerato de betametasona	13D03-N07	38
Fagron	Valerato de betametasona	13g19-n01	2
Fagron	Valerato de betametasona	13G19N01	1
Fagron	Valerato de betametasona	13G19-N01	49
Fagron	Valerato de betametasona	13G19-NO1	1
Fagron	Valerato de betametasona	13K05-B08	2
Fagron	Valerato de betametasona	13K05-B08-092652	1
Fagron	Valerato de betametasona	13K05-B08-291663	3
Fagron	Valerato de betametasona	13K05-B08-292647	2
Fagron	Valerato de betametasona	13K05-B08-292651	1
Fagron	Valerato de betametasona	13K05-B08-292652	2
Fagron	Valerato de betametasona	13K29-B12-288247	1
Fagron	Valerato de betametasona	13K29-B23-288246	1
Fagron	Valerato de betametasona	13K29B32	1
Fagron	Valerato de betametasona	13K29-B32	6
Fagron	Valerato de betametasona	13K29-B32-28824	1
Fagron	Valerato de betametasona	13K29B32288243	1
Fagron	Valerato de betametasona	13K29-B32-288244	2
Fagron	Valerato de betametasona	13K29-B32-288245	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	13K29-B32-288246	5
Fagron	Valerato de betametasona	13k29b32288247	1
Fagron	Valerato de betametasona	13K29-B32-288247	20
Fagron	Valerato de betametasona	13K29-B32-288248	3
Fagron	Valerato de betametasona	13K29-B32-288250	3
Fagron	Valerato de betametasona	13117-B08-292649	2
Fagron	Valerato de betametasona	1406019-03	1
Fagron	Valerato de betametasona	14188603	1
Fagron	Valerato de betametasona	14C19B02	1
Fagron	Valerato de betametasona	14C19-B02	3
Fagron	Valerato de betametasona	14C19-B02-292646	1
Fagron	Valerato de betametasona	14C19-B02-292648	1
Fagron	Valerato de betametasona	14c19-b02-292650	1
Fagron	Valerato de betametasona	14C19-B02-292650	4
Fagron	Valerato de betametasona	14C19-B02-292653	6
Fagron	Valerato de betametasona	14C19B02296168	1
Fagron	Valerato de betametasona	14C19-B02-296168	4
Fagron	Valerato de betametasona	14c19-b02-296169	1
Fagron	Valerato de betametasona	14C19-B02-296169	1
Fagron	Valerato de betametasona	14G30-B05	4
Fagron	Valerato de betametasona	14G30-B05-29617	1
Fagron	Valerato de betametasona	14G30-B05-296170	1
Fagron	Valerato de betametasona	14G30B05296172	1
Fagron	Valerato de betametasona	14G30-B05-296172	3
Fagron	Valerato de betametasona	14G30-B05-296173	14
Fagron	Valerato de betametasona	14G30-B05-296175	3
Fagron	Valerato de betametasona	14G30-B05-309518	2
Fagron	Valerato de betametasona	14G30B05309519	1
Fagron	Valerato de betametasona	14G30-B05-309519	1
Fagron	Valerato de betametasona	14G30-B05-309520	7
Fagron	Valerato de betametasona	14G30-B05-309521	1
Fagron	Valerato de betametasona	14G30-B05-309528	1
Fagron	Valerato de betametasona	14G30-Bo5-296172	1
Fagron	Valerato de betametasona	14G31-B04-342639	1
Fagron	Valerato de betametasona	14H28B01	1
Fagron	Valerato de betametasona	14H28-B01	3
Fagron	Valerato de betametasona	14H28-B01-302683	1
Fagron	Valerato de betametasona	14H28-B01-302863	5
Fagron	Valerato de betametasona	14H28B01302864	1
Fagron	Valerato de betametasona	14H28-B01-302864	6
Fagron	Valerato de betametasona	14H28-B01-302864/201	1
Fagron	Valerato de betametasona	14h28-b01-302865	2
Fagron	Valerato de betametasona	14H28-B01-302865	13
Fagron	Valerato de betametasona	14H28-b01-302866	1
Fagron	Valerato de betametasona	14H28-B01-302866	7
Fagron	Valerato de betametasona	14H28-B01-302877	3
Fagron	Valerato de betametasona	14H28-B01-305470	2
Fagron	Valerato de betametasona	15/16-B07	1
Fagron	Valerato de betametasona	15/16-B07-317416	5
Fagron	Valerato de betametasona	15/16-B07-317417	2
Fagron	Valerato de betametasona	15/16-B07-317428	3
Fagron	Valerato de betametasona	15/16-B07-319228	3
Fagron	Valerato de betametasona	15/16-B07-319831	1
Fagron	Valerato de betametasona	15/16-B07-319832	1
Fagron	Valerato de betametasona	15075802	1
Fagron	Valerato de betametasona	15116-B07	1
Fagron	Valerato de betametasona	1516-B07-317416	1
Fagron	Valerato de betametasona	1526260	1
Fagron	Valerato de betametasona	15398515	1
Fagron	Valerato de betametasona	15824-B04	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	15B24-B04	2
Fagron	Valerato de betametasona	15B24-B04-307015	4
Fagron	Valerato de betametasona	15B24-B04-307016	14
Fagron	Valerato de betametasona	15F16-804-314054	1
Fagron	Valerato de betametasona	15F16-B04	4
Fagron	Valerato de betametasona	15F16-B04-215327	1
Fagron	Valerato de betametasona	15f16-b04314054	1
Fagron	Valerato de betametasona	15F16-B04-314054	5
Fagron	Valerato de betametasona	15F16-B04-314054/201	1
Fagron	Valerato de betametasona	15F16-B04-314055	1
Fagron	Valerato de betametasona	15F16-B04-314882	1
Fagron	Valerato de betametasona	15F16-B04-315328	3
Fagron	Valerato de betametasona	15I16-B07	1
Fagron	Valerato de betametasona	15I16-B07-317416	1
Fagron	Valerato de betametasona	15I16B07317417	1
Fagron	Valerato de betametasona	15I16-B07-317417	1
Fagron	Valerato de betametasona	15I16-B07-319228	2
Fagron	Valerato de betametasona	15I16-B07-319832	3
Fagron	Valerato de betametasona	15I16-Bo7-319832	1
Fagron	Valerato de betametasona	15l16-B07-319832	2
Fagron	Valerato de betametasona	16270511	1
Fagron	Valerato de betametasona	16270513	1
Fagron	Valerato de betametasona	16818-B02-320971	1
Fagron	Valerato de betametasona	16818-B02-323033	1
Fagron	Valerato de betametasona	16B18_B02-322111	1
Fagron	Valerato de betametasona	16B18-B02	6
Fagron	Valerato de betametasona	16B18-B02-320606	1
Fagron	Valerato de betametasona	16B18B02320971	1
Fagron	Valerato de betametasona	16B18-B02320971	2
Fagron	Valerato de betametasona	16B18-B02-320971	6
Fagron	Valerato de betametasona	16B18-B02-322109	5
Fagron	Valerato de betametasona	16B18-B02-322111	2
Fagron	Valerato de betametasona	16B18-B02-322121	4
Fagron	Valerato de betametasona	16B18-B02-323033	1
Fagron	Valerato de betametasona	16b18-b02-323034	1
Fagron	Valerato de betametasona	16B18-B02-323034	4
Fagron	Valerato de betametasona	16b18-b02-324798	1
Fagron	Valerato de betametasona	16B18-B02-324798	3
Fagron	Valerato de betametasona	16E23-B03	8
Fagron	Valerato de betametasona	16E23-B03-324799	8
Fagron	Valerato de betametasona	16E23-B03-3247990855	1
Fagron	Valerato de betametasona	16e23b03324800	1
Fagron	Valerato de betametasona	16e23-b03-324800	1
Fagron	Valerato de betametasona	16E23-B03-324800	12
Fagron	Valerato de betametasona	16E23-B03-327350	5
Fagron	Valerato de betametasona	16E23-B03-327354	3
Fagron	Valerato de betametasona	16E23-b03-328128	1
Fagron	Valerato de betametasona	16E23B03328128	1
Fagron	Valerato de betametasona	16E23-B03-328128	10
Fagron	Valerato de betametasona	16E23-B03-328129	2
Fagron	Valerato de betametasona	16H22-B06	3
Fagron	Valerato de betametasona	16H22-B06-329223	6
Fagron	Valerato de betametasona	16H22-B06-329231	5
Fagron	Valerato de betametasona	16H22-B06-330522	2
Fagron	Valerato de betametasona	16h22-b06-330523	2
Fagron	Valerato de betametasona	16H22-B06-330523	4
Fagron	Valerato de betametasona	16H22B06330524	2
Fagron	Valerato de betametasona	16H22-B06-330524	6
Fagron	Valerato de betametasona	16h22b06330584	1
Fagron	Valerato de betametasona	16h22-b06-331273	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	16H22-B06-331273	1
Fagron	Valerato de betametasona	16H22-B06-332351	11
Fagron	Valerato de betametasona	16H22-B06-3332351	1
Fagron	Valerato de betametasona	170401901	1
Fagron	Valerato de betametasona	1704019-01	5
Fagron	Valerato de betametasona	17078701	1
Fagron	Valerato de betametasona	17271604	2
Fagron	Valerato de betametasona	17329001	1
Fagron	Valerato de betametasona	17329008	1
Fagron	Valerato de betametasona	17329016	1
Fagron	Valerato de betametasona	17B14-B04	1
Fagron	Valerato de betametasona	17C29-335654	1
Fagron	Valerato de betametasona	17C29-B04	7
Fagron	Valerato de betametasona	17C29-B04_336434	1
Fagron	Valerato de betametasona	17C29-B04-33368	1
Fagron	Valerato de betametasona	17C29-B04-333688	1
Fagron	Valerato de betametasona	17C29-B04-334329	10
Fagron	Valerato de betametasona	17c29-b04-335654	1
Fagron	Valerato de betametasona	17C29-B04-335654	3
Fagron	Valerato de betametasona	17c29-b04-335657	2
Fagron	Valerato de betametasona	17C29-B04-335657	11
Fagron	Valerato de betametasona	17C29B043356575581	1
Fagron	Valerato de betametasona	17C29-B04-335658	1
Fagron	Valerato de betametasona	17C29-B04-335676	6
Fagron	Valerato de betametasona	17C29-B04-336434	6
Fagron	Valerato de betametasona	17G31-B04	5
Fagron	Valerato de betametasona	17G31-B-04	1
Fagron	Valerato de betametasona	17g31-b04-338575	2
Fagron	Valerato de betametasona	17G31B04338575	1
Fagron	Valerato de betametasona	17G31-B04-338575	11
Fagron	Valerato de betametasona	17G31-B04-339784	15
Fagron	Valerato de betametasona	17G-31-B04-339784	1
Fagron	Valerato de betametasona	17G31B04339785	1
Fagron	Valerato de betametasona	17G31-B04-339785	4
Fagron	Valerato de betametasona	17G31-B04-341303	1
Fagron	Valerato de betametasona	17g31-b04-341576	3
Fagron	Valerato de betametasona	17G31B04341576	1
Fagron	Valerato de betametasona	17G31-B04-341576	12
Fagron	Valerato de betametasona	17G-31-B04-341576	1
Fagron	Valerato de betametasona	17G31-B04-341576-201	1
Fagron	Valerato de betametasona	17G31-B04-3415765	1
Fagron	Valerato de betametasona	17G31-B04-342639	1
Fagron	Valerato de betametasona	17G31-B04-344457	1
Fagron	Valerato de betametasona	17G31-B04-344757	2
Fagron	Valerato de betametasona	17K16_B08-348042	1
Fagron	Valerato de betametasona	17k16-b08	1
Fagron	Valerato de betametasona	17K16B08	1
Fagron	Valerato de betametasona	17K16-B08	11
Fagron	Valerato de betametasona	17K16-B08-344754	3
Fagron	Valerato de betametasona	17k16-b08-345541	4
Fagron	Valerato de betametasona	17K16-B08-345541	11
Fagron	Valerato de betametasona	17K16-B08-345542	1
Fagron	Valerato de betametasona	17K16-B08-345555	5
Fagron	Valerato de betametasona	17k16-B08-347309	1
Fagron	Valerato de betametasona	17K16-B08-347309	9
Fagron	Valerato de betametasona	17K-16-B08-347309	2
Fagron	Valerato de betametasona	17k16-b08-347310	1
Fagron	Valerato de betametasona	17K16-B08-347310	4
Fagron	Valerato de betametasona	17k16-b08-347912	1
Fagron	Valerato de betametasona	17k16-B08-347912	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	17K16-B08-347912	10
Fagron	Valerato de betametasona	17K16-B08-348042	14
Fagron	Valerato de betametasona	17K16-B08-348538	2
Fagron	Valerato de betametasona	17K16-B08-349755	9
Fagron	Valerato de betametasona	17K16-B08-349774	1
Fagron	Valerato de betametasona	17K16-B09-345541	1
Fagron	Valerato de betametasona	17k16-bo8-347309	1
Fagron	Valerato de betametasona	17K16-B0B-345541	1
Fagron	Valerato de betametasona	18/26-B05-356852	1
Fagron	Valerato de betametasona	18/27-B05	1
Fagron	Valerato de betametasona	18/27-B05-354880	1
Fagron	Valerato de betametasona	18/27-B05-356570	1
Fagron	Valerato de betametasona	18/27-B05-356571	4
Fagron	Valerato de betametasona	18/27-B05-356584	1
Fagron	Valerato de betametasona	18/27-b05-357770	1
Fagron	Valerato de betametasona	18/27-B05-357770	1
Fagron	Valerato de betametasona	18/27-B05-358065	4
Fagron	Valerato de betametasona	18/27-B05-360081	1
Fagron	Valerato de betametasona	18/27-B05-356570	1
Fagron	Valerato de betametasona	1811008-01	1
Fagron	Valerato de betametasona	18127-B05-358065	1
Fagron	Valerato de betametasona	1817-B05-360082	1
Fagron	Valerato de betametasona	18199907	1
Fagron	Valerato de betametasona	18G03-03-351731	1
Fagron	Valerato de betametasona	18G03-B03	6
Fagron	Valerato de betametasona	18G03-B03_351731	1
Fagron	Valerato de betametasona	18G03-B03-351450	12
Fagron	Valerato de betametasona	18G03-B03-351451	1
Fagron	Valerato de betametasona	18G03-B03-351513	3
Fagron	Valerato de betametasona	18G03-B03-351730	2
Fagron	Valerato de betametasona	18G03-B03-351731	21
Fagron	Valerato de betametasona	18G03-B03-351731	1
Fagron	Valerato de betametasona	18G03-B03-352458	1
Fagron	Valerato de betametasona	18G03-B03-352460	7
Fagron	Valerato de betametasona	18G03-B03-353212	13
Fagron	Valerato de betametasona	18I07-B05-356584	1
Fagron	Valerato de betametasona	18I27-B05	3
Fagron	Valerato de betametasona	18I27-B05_356571	1
Fagron	Valerato de betametasona	18I27-B05-354898	1
Fagron	Valerato de betametasona	18I27-B05-356570	2
Fagron	Valerato de betametasona	18i27B05356571	1
Fagron	Valerato de betametasona	18I27-B05356571	1
Fagron	Valerato de betametasona	18I27-B05-356571	5
Fagron	Valerato de betametasona	18I27-B05-356852	1
Fagron	Valerato de betametasona	18I27-B05-357770	2
Fagron	Valerato de betametasona	18I27-b05-358065	1
Fagron	Valerato de betametasona	18I27-B05-358065	5
Fagron	Valerato de betametasona	18I27-B5-356571	1
Fagron	Valerato de betametasona	18127-B05	1
Fagron	Valerato de betametasona	18127-B05-356584	1
Fagron	Valerato de betametasona	18127-B05-357770	1
Fagron	Valerato de betametasona	19/26-F02-364980	1
Fagron	Valerato de betametasona	19/26-F02-364981	2
Fagron	Valerato de betametasona	19126-F02-364980	1
Fagron	Valerato de betametasona	19G03-B02-363670	1
Fagron	Valerato de betametasona	19G30-B02	17
Fagron	Valerato de betametasona	19G30B02363672	1
Fagron	Valerato de betametasona	19G30-B02-363672	8
Fagron	Valerato de betametasona	19g30-b02-363673	1
Fagron	Valerato de betametasona	19G30-B02-363673	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	19G30-B02-363681	1
Fagron	Valerato de betametasona	19g30-b02-363682	1
Fagron	Valerato de betametasona	19G30-B02-363682	17
Fagron	Valerato de betametasona	19G30-B02-363686	5
Fagron	Valerato de betametasona	19G30-B02-363692	8
Fagron	Valerato de betametasona	19G30-B02-363693	15
Fagron	Valerato de betametasona	19G30-B03-363692	1
Fagron	Valerato de betametasona	19G30-Bo2-363693	1
Fagron	Valerato de betametasona	19GB0-B02-363693	1
Fagron	Valerato de betametasona	19I26-F02	4
Fagron	Valerato de betametasona	19I26F02364980	1
Fagron	Valerato de betametasona	19I26-F02-364980	4
Fagron	Valerato de betametasona	19I26-F02-364981	6
Fagron	Valerato de betametasona	19I26-F02-364982	1
Fagron	Valerato de betametasona	19I26-F02-364987	6
Fagron	Valerato de betametasona	19I86-F02-364987	1
Fagron	Valerato de betametasona	19J26-F02-364987	1
Fagron	Valerato de betametasona	19K11-07-366784	1
Fagron	Valerato de betametasona	19K11-F07	7
Fagron	Valerato de betametasona	19K11-F07-366779	3
Fagron	Valerato de betametasona	19k11-f07-366780	1
Fagron	Valerato de betametasona	19K11-F07-366780	1
Fagron	Valerato de betametasona	19K11-F07-3667807	1
Fagron	Valerato de betametasona	19K11-F07-3667809	1
Fagron	Valerato de betametasona	19K11-F07-366782	1
Fagron	Valerato de betametasona	19K11-F07-366784	1
Fagron	Valerato de betametasona	19k11-F07-366785	1
Fagron	Valerato de betametasona	19K11-F07-366785	16
Fagron	Valerato de betametasona	19k11f07366786	1
Fagron	Valerato de betametasona	19K11-F07-366786	9
Fagron	Valerato de betametasona	19K11-F07-366787	5
Fagron	Valerato de betametasona	19K11-F07-366788	3
Fagron	Valerato de betametasona	19K11-F07-366788	1
Fagron	Valerato de betametasona	19K11-F07-366789	3
Fagron	Valerato de betametasona	19K11-Fo7-366785	1
Fagron	Valerato de betametasona	19K11-F07-366785	1
Fagron	Valerato de betametasona	19K-F0-366786	1
Fagron	Valerato de betametasona	19126-F02	3
Fagron	Valerato de betametasona	19126-F02-364981	1
Fagron	Valerato de betametasona	19126-F02-364986	1
Fagron	Valerato de betametasona	19UI26-F02-364981	1
Fagron	Valerato de betametasona	2000036016	1
Fagron	Valerato de betametasona	20101012-1	1
Fagron	Valerato de betametasona	20818-F07	1
Fagron	Valerato de betametasona	20B18-F07	5
Fagron	Valerato de betametasona	20B18-F07-3696704	2
Fagron	Valerato de betametasona	20B18-F07-369671	2
Fagron	Valerato de betametasona	20B18-F07-369673	17
Fagron	Valerato de betametasona	20B18-F07-369674	1
Fagron	Valerato de betametasona	20B18-F07-369676	3
Fagron	Valerato de betametasona	20B18-F07-3700009	1
Fagron	Valerato de betametasona	20B18-F07-370009	6
Fagron	Valerato de betametasona	20B18-F07-370010	2
Fagron	Valerato de betametasona	20B18F07370013	1
Fagron	Valerato de betametasona	20B18-F07-370013	3
Fagron	Valerato de betametasona	20B18-F07-37009	1
Fagron	Valerato de betametasona	20E14-F02	3
Fagron	Valerato de betametasona	20E14-F02-371690	13
Fagron	Valerato de betametasona	20E14-F02-372350	7
Fagron	Valerato de betametasona	20G17-F02	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	20G17-F02-3737909	1
Fagron	Valerato de betametasona	20G17-F02-373798	7
Fagron	Valerato de betametasona	20G17-F02-373799	5
Fagron	Valerato de betametasona	21000036020	1
Fagron	Valerato de betametasona	2152-44-5	1
Fagron	Valerato de betametasona	21D09-F03	3
Fagron	Valerato de betametasona	21D09-F03-377824	7
Fagron	Valerato de betametasona	21D09-F03-377825	4
Fagron	Valerato de betametasona	21D09-F03377843	1
Fagron	Valerato de betametasona	21D09-F03-377843	1
Fagron	Valerato de betametasona	21G28-B02	1
Fagron	Valerato de betametasona	21G28-B02-213513	1
Fagron	Valerato de betametasona	21G28-B02-213516	9
Fagron	Valerato de betametasona	21G28-B02-213517	4
Fagron	Valerato de betametasona	21G28-B02-213518	6
Fagron	Valerato de betametasona	21G28-B02-213663	2
Fagron	Valerato de betametasona	21G28-BO2-213518	1
Fagron	Valerato de betametasona	21K09_B05_218135	1
Fagron	Valerato de betametasona	21K09B05	1
Fagron	Valerato de betametasona	21K09-B05	1
Fagron	Valerato de betametasona	21K09-B05-217883	8
Fagron	Valerato de betametasona	21K09B05217891	1
Fagron	Valerato de betametasona	21K09-B05-217891	8
Fagron	Valerato de betametasona	21K09-B05-217898	2
Fagron	Valerato de betametasona	21K09-B05-218135	1
Fagron	Valerato de betametasona	21K09-B05-220180	7
Fagron	Valerato de betametasona	21K09B05220215	1
Fagron	Valerato de betametasona	21K09-B05-220215	5
Fagron	Valerato de betametasona	21K09-B05-220334	1
Fagron	Valerato de betametasona	21K09-B05-220365	2
Fagron	Valerato de betametasona	21K09-B05-2221193	1
Fagron	Valerato de betametasona	21K09-B05-222192	4
Fagron	Valerato de betametasona	21K09-B05-222194	1
Fagron	Valerato de betametasona	22H25B07	1
Fagron	Valerato de betametasona	22H25-B07	1
Fagron	Valerato de betametasona	22H25B07223527	4
Fagron	Valerato de betametasona	22H25-B07-223527	4
Fagron	Valerato de betametasona	22H25-B07-223537	1
Fagron	Valerato de betametasona	22H25B072235527	1
Fagron	Valerato de betametasona	292652	1
Fagron	Valerato de betametasona	2B28-N01	1
Fagron	Valerato de betametasona	2OB18-F07-370009	1
Fagron	Valerato de betametasona	309520	1
Fagron	Valerato de betametasona	364979	1
Fagron	Valerato de betametasona	612211181	1
Fagron	Valerato de betametasona	700103-0002	3
Fagron	Valerato de betametasona	700103-0003	1
Fagron	Valerato de betametasona	700103-0004	2
Fagron	Valerato de betametasona	90616-2	1
Fagron	Valerato de betametasona	B02-3636307	1
Fagron	Valerato de betametasona	b02-3636702	1
Fagron	Valerato de betametasona	B02-3636802	1
Fagron	Valerato de betametasona	B05-217898	1
Fagron	Valerato de betametasona	B05-2203305	1
Fagron	Valerato de betametasona	B07-317416	1
Fagron	Valerato de betametasona	BO5-2203305	1
Fagron	Valerato de betametasona	BV004/0721	2
Fagron	Valerato de betametasona	BV008/0415	1
Fagron	Valerato de betametasona	BV008/045	1
Fagron	Valerato de betametasona	BV008/0516	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de betametasona	BV009/0117	1
Fagron	Valerato de betametasona	BV019/0514	3
Fagron	Valerato de betametasona	BV036/1215	1
Fagron	Valerato de betametasona	BV102/0420	6
Fagron	Valerato de betametasona	BV106/0717	2
Fagron	Valerato de betametasona	BV109/0117	2
Fagron	Valerato de betametasona	BV109/0519	6
Fagron	Valerato de betametasona	BV110/0818	1
Fagron	Valerato de betametasona	BV123/0120	2
Fagron	Valerato de betametasona	BV124/0118	2
Fagron	Valerato de betametasona	BV127/0120	1
Fagron	Valerato de betametasona	BV-BLT225/0514	1
Fagron	Valerato de betametasona	BV-BLT250/0616	2
Fagron	Valerato de betametasona	F02-3649807	2
Fagron	Valerato de betametasona	F02-3716900	1
Fagron	Valerato de betametasona	F02-3723500	1
Fagron	Valerato de betametasona	F02-3737908	1
Fagron	Valerato de betametasona	F02-3737909	2
Fagron	Valerato de betametasona	F03377824	1
Fagron	Valerato de betametasona	F07-3667805	1
Fagron	Valerato de betametasona	F07-3667808	1
Fagron	Valerato de betametasona	F07-3696703	1
Fagron	Valerato de betametasona	F07-3700100	1
Fagron	Valerato de betametasona	F073700103	1
Fagron	Valerato de betametasona	fagron	1
Fagron	Valerato de betametasona	NP1351M	1
Fagron	Valerato de betametasona	NS0706M	3
Fagron	Valerato de betametasona	NS2072M	1
Fagron	Valerato de betametasona	NT0597M	4
Fagron	Valerato de betametasona	NT059M	1
Fagron	Valerato de betametasona	Op07062022B	1
Fargon, Noweda 07.11.2017	Valerato de betametasona	16H22-B06-329223	1
Fargon/AHD	Valerato de betametasona	18/27-B05	1
Fargon/Alliance HC	Valerato de betametasona	13K29-B32-288247	1
Fargon/Alliance HC	Valerato de betametasona	16B18-B02-322111	1
Fargon/Anzag	Valerato de betametasona	13G19-N01	1
Fargon/Anzag	Valerato de betametasona	16B18-B02-320971	1
Fargon/Noweda	Valerato de betametasona	18I27-B05-354898	1
Fargon	Valerato de betametasona	13k29-b32-289364	1
Fargon	Valerato de betametasona	18g03-b03-351731	1
Fargon	Valerato de betametasona	19G30-B08-36393	1
Fargon	Valerato de betametasona	20G17-F02-373798	1
Fargon	Valerato de betametasona	21K09-B05-217883	1
Fargon	Valerato de betametasona	7890	1
Fargron	Valerato de betametasona	13G19-N01	1
Fargron	Valerato de betametasona	13K29-B32-288246	1
Farmabios S. p. A./ …	Valerato de betametasona	17078715	1
Farmabios S.p.A., IT	Valerato de betametasona	2109VM00012222	1
Farmabios spa	Valerato de betametasona	19220704	1
Farmabios/Noweda	Valerato de betametasona	2109VM0B0011722	1
Farmabios/Noweda	Valerato de betametasona	2109VMOB0011722	1
Farmabios/Phoenix	Valerato de betametasona	2109VMOCO011922	1
Farmabios	Valerato de betametasona	17271603	1
Fiebig 27.06.13 EK47,81	Valerato de betametasona	B9/131	1
Fiebig ek: 45,65EUR	Valerato de betametasona	12B28-N01	1
Fiebig/Farago	Valerato de betametasona	19G30-B02-363692	1
Fiebig	Valerato de betametasona	14H28-B01	1
Fiebig	Valerato de betametasona	15B24-B04-307016	1
Fiebig	Valerato de betametasona	16B18-B02-322111	1
Fiebig	Valerato de betametasona	17271603	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
FIEBIG	Valerato de betametasona	F17-3696703	1
Finteler Apotheke	Valerato de betametasona	17C29-B04-333688	2
Fragon/ Gehe	Valerato de betametasona	19K11-F07-366785	1
Fragon/Alliance	Valerato de betametasona	17k16-B08	1
Fragon/Phönix	Valerato de betametasona	17G31-B04-341576	1
Fragon/Sanacorp	Valerato de betametasona	17K16-B08-340842	1
Fragon	Valerato de betametasona	16G03-B03-353212	1
Fragon	Valerato de betametasona	19K11-F07-366784	1
Fragron	Valerato de betametasona	BV-BLT225/0514	2
Galderma/ Noweda	Valerato de betametasona	C0023/115040	1
Gatt-Koller	Valerato de betametasona	1800117	1
GEHE 17.06.2014	Valerato de betametasona	13225503	1
Gehe am 03.02.2014	Valerato de betametasona	13091210	3
Gehe amax	Valerato de betametasona	18199930	1
Gehe	Valerato de betametasona	12003403	1
Gehe	Valerato de betametasona	12003409	1
Gehe	Valerato de betametasona	1208014-04	1
Gehe	Valerato de betametasona	12229809	1
Gehe	Valerato de betametasona	13091211	1
Gehe	Valerato de betametasona	14H25-B01-302863	1
Gehe	Valerato de betametasona	14H28-B01-302863	1
Gehe	Valerato de betametasona	15075804	1
Gehe	Valerato de betametasona	15075811	1
Gehe	Valerato de betametasona	15398501	1
Gehe	Valerato de betametasona	15398512	1
GEHE	Valerato de betametasona	16270501	1
Gehe	Valerato de betametasona	16270505	1
Gehe	Valerato de betametasona	16H22-B06	1
Gehe	Valerato de betametasona	16H22-B06-330524	1
GEHE	Valerato de betametasona	17078701	2
Gehe	Valerato de betametasona	17078703	1
Gehe	Valerato de betametasona	17078712	1
GEHE	Valerato de betametasona	17078719	1
GEHE	Valerato de betametasona	17078720	1
Gehe	Valerato de betametasona	1712E-01181	1
Gehe	Valerato de betametasona	17271603	1
Gehe	Valerato de betametasona	17329015	1
Gehe	Valerato de betametasona	17329018	1
Gehe	Valerato de betametasona	17G31-B04	1
Gehe	Valerato de betametasona	17K16-B08	1
Gehe	Valerato de betametasona	17K16-B08-347309	1
Gehe	Valerato de betametasona	17K16-B08-348042	1
Gehe	Valerato de betametasona	1811008-01	1
GEHE	Valerato de betametasona	18199902	2
Gehe	Valerato de betametasona	18199908	1
Gehe	Valerato de betametasona	18199924	3
gehe	Valerato de betametasona	18199937	1
Gehe	Valerato de betametasona	18G03-B03-351731	1
Gehe	Valerato de betametasona	18I27-B05	1
Gehe	Valerato de betametasona	192207001	2
Gehe	Valerato de betametasona	192207002	1
Gehe	Valerato de betametasona	19220702	1
Gehe	Valerato de betametasona	21K09-b05	1
gehe	Valerato de betametasona	21K09-B05-220180	1
Gehe	Valerato de betametasona	21K09-B05-22192	1
GEHE	Valerato de betametasona	22001101015	1
Gehe	Valerato de betametasona	22001101016	1
Gehe	Valerato de betametasona	22001101021	1
Gehe	Valerato de betametasona	2202016-01	2
Gehe	Valerato de betametasona	2202016-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
gehe	Valerato de betametasona	22H25B07227237	1
Gehe	Valerato de betametasona	22K07-B08-229283	1
Gehe	Valerato de betametasona	22K07-B08-233606	1
Gehe	Valerato de betametasona	2309023-01	1
Gehe	Valerato de betametasona	23E29-B03-235955	1
Gehe	Valerato de betametasona	23E29-B03-238320	1
Gehe	Valerato de betametasona	BV001/0322	1
Geilenkirchen	Valerato de betametasona	16270513	1
Geilenkirchen	Valerato de betametasona	17078701	1
Geilenkirchen	Valerato de betametasona	18199918	1
Hedinger / Noweda	Valerato de betametasona	16270505	1
Hedinger	Valerato de betametasona	14H28-B01-302877	1
Hepart AG, CH-8280 K...	Valerato de betametasona	11131914	3
Hirsch	Valerato de betametasona	13G19-No1	1
Holdermann	Valerato de betametasona	1208014-01	1
Holdermann	Valerato de betametasona	120801402	1
Ichthyol-Gesellschaft	Valerato de betametasona	13k29-B32-288247	1
Ichthyol-Gesellschaft	Valerato de betametasona	17078720	1
jenne/eurho	Valerato de betametasona	2102010-01	1
Jenne	Valerato de betametasona	17078712	1
Jenne	Valerato de betametasona	1811008-01	3
Jenne	Valerato de betametasona	18199918	1
Jenne	Valerato de betametasona	18199933	1
Jenne	Valerato de betametasona	18I27-B05-358065	1
Jenne	Valerato de betametasona	21000036017	1
Jenne	Valerato de betametasona	22001101004	1
Jenne	Valerato de betametasona	22001101020	1
Kehr	Valerato de betametasona	1801024-01	1
Kehr	Valerato de betametasona	22001101015	1
Kehr	Valerato de betametasona	22001101020	1
Kehr	Valerato de betametasona	2202016-01	1
Kehr	Valerato de betametasona	22H25-07-227224	1
Klenk	Valerato de betametasona	16623-01	1
Klenk	Valerato de betametasona	17078713	1
Klenk	Valerato de betametasona	17078714	1
Klosterring	Valerato de betametasona	18199916	2
Krieger	Valerato de betametasona	192207010	1
krieger	Valerato de betametasona	20G17-F02-373798	1
L12	Valerato de betametasona	16E23-B03-324799	2
L12	Valerato de betametasona	17C29-B04-334329	2
L12	Valerato de betametasona	17K16-B08-345541	1
Lamotte/Noweda	Valerato de betametasona	17K16-B08-349755	1
Midas	Valerato de betametasona	16270503	1
Midas	Valerato de betametasona	16270513	1
Midas	Valerato de betametasona	17078712	2
Midas	Valerato de betametasona	17078720	1
Midas	Valerato de betametasona	17329001	2
Midas	Valerato de betametasona	17329018	1
Midas	Valerato de betametasona	17G31-B04-338575	2
Mömerzheim	Valerato de betametasona	17329008	1
NEWCHEM	Valerato de betametasona	1311039-01	1
Noveda	Valerato de betametasona	1311039-01	1
Noveda	Valerato de betametasona	192207002	1
Noweda/ Infecto Pharm	Valerato de betametasona	16270505	1
Noweda/cealo	Valerato de betametasona	17329002	1
Noweda/Ceasar Lorenz	Valerato de betametasona	14188606	1
Noweda	Valerato de betametasona	11131902	1
Noweda	Valerato de betametasona	11B21-N02	1
Noweda	Valerato de betametasona	1208014-01	1
Noweda	Valerato de betametasona	1208014-02	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
noweda	Valerato de betametasona	1208014-04	1
Noweda	Valerato de betametasona	12229832	1
Noweda	Valerato de betametasona	12G09-N07	1
Noweda	Valerato de betametasona	13091203	1
Noweda	Valerato de betametasona	13091205	1
noweda	Valerato de betametasona	1406019-01	1
Noweda	Valerato de betametasona	1406019-03	2
Noweda	Valerato de betametasona	14H28B01302863	1
Noweda	Valerato de betametasona	15075812	1
Noweda	Valerato de betametasona	161001001	1
Noweda	Valerato de betametasona	16270511	1
Noweda	Valerato de betametasona	1704019-01	1
Noweda	Valerato de betametasona	17078701	1
Noweda	Valerato de betametasona	17271601	2
Noweda	Valerato de betametasona	17329018	2
Noweda	Valerato de betametasona	17g31-b04-338575	1
Noweda	Valerato de betametasona	1801024-01	2
Noweda	Valerato de betametasona	1811008-01	2
Noweda	Valerato de betametasona	18199918	1
Noweda	Valerato de betametasona	18199932	3
Noweda	Valerato de betametasona	18199933	1
Noweda	Valerato de betametasona	18127-B05-354880	1
Noweda	Valerato de betametasona	1912012-01	1
Noweda	Valerato de betametasona	19220704	2
Noweda	Valerato de betametasona	19220705	2
Noweda	Valerato de betametasona	19I26-F02-364981	1
Noweda	Valerato de betametasona	20G17-F02-373798	1
Noweda	Valerato de betametasona	21000036003	1
Noweda	Valerato de betametasona	21K09-B05	1
Noweda	Valerato de betametasona	22001101003	1
Noweda	Valerato de betametasona	2202016-01	6
Noweda	Valerato de betametasona	22K07-08-229283	1
Noweda	Valerato de betametasona	2309023	1
Noweda	Valerato de betametasona	2309023-01	2
Noweda	Valerato de betametasona	BV01090117	1
Oberlinden- Apotheke	Valerato de betametasona	C0073/1	3
Oberlinden Apotheke	Valerato de betametasona	C0073/115040	3
Oberlinden Apotheke	Valerato de betametasona	c073/115040	1
Phoenix 15.1.2014	Valerato de betametasona	1208014-04	1
Phoenix 13.12.2017	Valerato de betametasona	16H22-B06-330524	1
Phoenix 22.01.2019	Valerato de betametasona	1801021-01	1
Phoenix 30.10.19 19,34EUR	Valerato de betametasona	18/27-B05-358065	1
Phoenix Goettin	Valerato de betametasona	13225508	1
Phoenix/ Fagro	Valerato de betametasona	18G03-B03-351731	1
Phoenix	Valerato de betametasona	12003409	2
Phoenix	Valerato de betametasona	16270513	1
Phoenix	Valerato de betametasona	170401901	1
Phoenix	Valerato de betametasona	17329002	1
Phoenix	Valerato de betametasona	17329018	1
Phoenix	Valerato de betametasona	17C29-B04-334329	1
Phoenix	Valerato de betametasona	17K16-B08-348042	2
Phoenix	Valerato de betametasona	1801024-01	1
Phoenix	Valerato de betametasona	1811008-01	2
Phoenix	Valerato de betametasona	18127-B05-358065	1
Phoenix	Valerato de betametasona	191201201	1
Phoenix	Valerato de betametasona	192207003	1
Phoenix	Valerato de betametasona	192207009	1
Phoenix	Valerato de betametasona	19220705	1
Phoenix	Valerato de betametasona	19G30-B02-363672	2
Phoenix	Valerato de betametasona	19G30-B02-363682	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Valerato de betametasona	19K11-F07	1
Phoenix	Valerato de betametasona	19126-F02-3649800	1
Phoenix	Valerato de betametasona	200592406	1
Phoenix	Valerato de betametasona	2102010-01	1
Phoenix	Valerato de betametasona	22001101016	2
Phoenix	Valerato de betametasona	3105	1
Phoenix	Valerato de betametasona	3364	1
Phönix Gotha	Valerato de betametasona	12229808	1
Phönix Gotha	Valerato de betametasona	13091213	1
Phönix Gotha	Valerato de betametasona	14188608	1
Phönix Gotha	Valerato de betametasona	1704019-01	1
Phönix Gotha	Valerato de betametasona	1811008-01	1
Phönix WE:16.07.2016...	Valerato de betametasona	1510037-01	1
Phönix	Valerato de betametasona	12229807	1
Phönix	Valerato de betametasona	13091201	2
Phönix	Valerato de betametasona	13091209	2
Phönix	Valerato de betametasona	13091212	2
Phönix	Valerato de betametasona	13D03-N07	1
Phonix	Valerato de betametasona	13K29-B32	1
phönix	Valerato de betametasona	15/16B07-319228	1
Phönix	Valerato de betametasona	15075804	1
Phönix	Valerato de betametasona	1507804	1
phönix	Valerato de betametasona	15398515	1
Phönix	Valerato de betametasona	16270503	1
phönix	Valerato de betametasona	16e23-b03-327350	1
Phönix	Valerato de betametasona	16H22-B06-330522	1
Phönix	Valerato de betametasona	17078712	1
Phönix	Valerato de betametasona	17329001	1
Phönix	Valerato de betametasona	18199907	1
Phönix	Valerato de betametasona	18199918	1
Phönix	Valerato de betametasona	18199933	1
Phönix	Valerato de betametasona	1911001-01	2
Phönix	Valerato de betametasona	192207009	1
Phönix	Valerato de betametasona	19220705	1
Phönix	Valerato de betametasona	19g30-b02-363672	1
Phönix	Valerato de betametasona	19G30-B02-363693	1
Phönix	Valerato de betametasona	19I26-F02-0364979	2
Phönix	Valerato de betametasona	19I26-F02-364981	1
Phönix	Valerato de betametasona	19K11-F07-366779	1
PHÖNIX	Valerato de betametasona	19K11-F07-366785	1
Phönix	Valerato de betametasona	19K11-F07-366786	1
Phönix	Valerato de betametasona	19K11-F07-366787	2
Phönix	Valerato de betametasona	19K11-F07-366789	1
Phönix	Valerato de betametasona	20E14-F02-371690	1
Phönix	Valerato de betametasona	21K09-B05-220215	1
Phönix	Valerato de betametasona	22001101009	1
Phönix	Valerato de betametasona	22001101018	1
Phönix	Valerato de betametasona	22001101020	2
Phönix	Valerato de betametasona	22001101021	1
Phönix	Valerato de betametasona	2202016-02	1
Phönix	Valerato de betametasona	B02-3636802	1
Phönix	Valerato de betametasona	BV110/0818	1
Phönix	Valerato de betametasona	BV-BLT186/0512	1
Phönix	Valerato de betametasona	F07-3696701	1
Röntgen	Valerato de betametasona	1911001-01	4
Sanacorp W.E: 18.01....	Valerato de betametasona	1704019-01	1
Sanacorp	Valerato de betametasona		1
Sanacorp	Valerato de betametasona	12G09-N07	1
Sanacorp	Valerato de betametasona	13091210	1
Sanacorp	Valerato de betametasona	13225503	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Valerato de betametasona	14188602	1
Sanacorp	Valerato de betametasona	14G30-B05-296173	1
Sanacorp	Valerato de betametasona	16H22-B06-330522	1
Sanacorp	Valerato de betametasona	1704019-01	1
Sanacorp	Valerato de betametasona	17078715	1
Sanacorp	Valerato de betametasona	17078719	1
Sanacorp	Valerato de betametasona	17C29-B04	1
Sanacorp	Valerato de betametasona	1801024-01	4
Sanacorp	Valerato de betametasona	1811008	2
Sanacorp	Valerato de betametasona	1811008-01	7
Sanacorp	Valerato de betametasona	18199918	2
Sanacorp	Valerato de betametasona	18199933	3
Sanacorp	Valerato de betametasona	192207010	1
Sanacorp	Valerato de betametasona	19220705	1
Sanacorp	Valerato de betametasona	19G30-B02-3636706	1
Sanacorp	Valerato de betametasona	19G30-B02-3636806	1
Sanacorp	Valerato de betametasona	19I26f02364981	1
Sanacorp	Valerato de betametasona	21000036017	1
Sanacorp	Valerato de betametasona	2100036021	1
Sanacorp	Valerato de betametasona	2102010-02	1
Sanacorp	Valerato de betametasona	22K07-B08-233606	1
Sanacorp	Valerato de betametasona	30051201	1
Sanacorp	Valerato de betametasona	F07-3700100	1
Spangro 31.05.2013	Valerato de betametasona	13D03-N07	2
Spangro	Valerato de betametasona	17078714	1
Spangro_21.05.2019	Valerato de betametasona	1811008-01	3
Symbiotica / Gehe	Valerato de betametasona	BV018/0715	1
Symbiotica / Gehe	Valerato de betametasona	BV036/1215	1
Symbiotica / Sanacorp	Valerato de betametasona	18I27-B05-354898	2
Symbiotica Spec.	Valerato de betametasona	1208014-04	1
Symbiotica Spec.	Valerato de betametasona	1406019-01	3
Symbiotica/ Anzag	Valerato de betametasona	1606023-01	2
Symbiotica/ Phönix	Valerato de betametasona	2102010-01	3
Symbiotica/Gehe	Valerato de betametasona	1912012-01	1
Symbiotica	Valerato de betametasona	14H28B01302863	1
Symbiotica	Valerato de betametasona	1610010-01	2
Symbotica Spec/Noweda	Valerato de betametasona	1208014-04	1
vdl	Valerato de betametasona	12003411	1

- 230 446 spectra from 1515 *Apo-Ident* customers from a total of 48 411 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Valerato de betametasona* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Valerato de betametasona* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	554	0	152 408
Type B	0	881	0	201 203
Type C	0	5546	75	230 446

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

The substance/substance group *Valerato de betametasona* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9170 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3190 %)
Type C	100.0000 % (> 99.9007 %)	98.6657 % (> 98.6123 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20887	22249	8,97	103,83
20920	22249	10,19	115,83
21215	22249	8,68	115,14
21566	22249	7,71	113,56
21588	21588	0,00	109,14
21645	22249	6,83	110,85
21674	21674	0,00	142,65
22249	22249	0,00	111,36
22861	22861	0,00	114,47
24349	24349	0,00	106,58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Valerato de estradiol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20330-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Valerato de estradiol; Estradiol, valerato; Estradioli valeras

Special notes

When selecting the *Valerato de estradiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Valerato de estradiol	6	4	137

Second-stage model

For differentiation of the substance/substance group *Valerato de estradiol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Valerato de estradiol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	90,34	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Valerato de estradiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Valerato de estradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Valerato de estradiol	13264001	21411	60	1410503
Caelo	Valerato de estradiol	13264001	21411SI	45	1410503
Caelo	Valerato de estradiol	13264001	21416	120	1510624
Caelo	Valerato de estradiol	13264001	21416SI	45	1510624
Caelo	Valerato de estradiol	13264001	21417	20	20130920
Caelo	Valerato de estradiol	13264001	21418	20	20130920
Caelo	Valerato de estradiol	13264001	21419	20	20130920
Caelo	Valerato de estradiol	13264001	21422	20	20130920
Caelo	Valerato de estradiol	13264001	21423	20	20130920
Caelo	Valerato de estradiol	13264001	21424	60	1410503
Caelo	Valerato de estradiol	13264001	21425	20	20130920
Caelo	Valerato de estradiol	13264001	21426	20	20130920
Caelo	Valerato de estradiol	15194802	21989	60	20150708
Caelo	Valerato de estradiol	15194802	21989SI	30	20150708
Caelo	Valerato de estradiol	163277	23056	40	20161221*
Caelo	Valerato de estradiol	163277	23056SI	40	20161221*
Caelo	Valerato de estradiol	22000384013	26741	40	20220407
Fagron	Valerato de estradiol	12D18-N02	20651	40	20120426
Fagron	Valerato de estradiol	12D18-N02	21266	40	20120118
Fagron	Valerato de estradiol	14E26-B02-294846	21646	60	20140616

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 820 spectra of 20 reference samples from the substance/substance group *Valerato de estradiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 142 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 467 spectra of 16 reference samples from the substance/substance group *Valerato de estradiol*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Valerato de estradiol	180674	24030	40
Caelo	Valerato de estradiol	20002389004	25427	40
Caelo	Valerato de estradiol	24000954	27231	40
Fagron	Valerato de estradiol	20J16-F01-375199	25753	40
Caelo	Valerato de estradiol	13264001	21417SI†	14
Caelo	Valerato de estradiol	13264001	21418SI†	15
Caelo	Valerato de estradiol	13264001	21419SI†	15
Caelo	Valerato de estradiol	13264001	21422SI†	17
Caelo	Valerato de estradiol	13264001	21423SI†	15
Caelo	Valerato de estradiol	13264001	21425SI†	15
Caelo	Valerato de estradiol	13264001	21426SI†	16
Caelo	Valerato de estradiol	180674	24030SI	40
Caelo	Valerato de estradiol	20002389004	25427SI	40
Caelo	Valerato de estradiol	22000384013	26741SI†	40
Caelo	Valerato de estradiol	24000954	27231SI	40
Fagron	Valerato de estradiol	20J16-F01-375199	25753SI	40

- 201 617 spectra from a total of 4039 batches from further 842 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 500 spectra from 207 *Apo-Ident* customers from 147 batches from the substance/substance group *Valerato de estradiol*.
- Among them are spectra of independent samples from 137 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Valerato de estradiol	22000384002	1
	Valerato de estradiol	22000384007	1
	Valerato de estradiol	22000384010	2
	Valerato de estradiol	22000384011	3
	Valerato de estradiol	22000384015	4
	Valerato de estradiol	22000384017	2
	Valerato de estradiol	22000384021	1
	Valerato de estradiol	ESV003-1A	1
	Valerato de estradiol	F01-3760807	1
Bayer Pharma / Gehe	Valerato de estradiol	84404140	1
Bayer Pharma AG	Valerato de estradiol	15C10-B05-305395	1
Bayer Pharma GmbH	Valerato de estradiol	82201620	1
Beiersdorf/AHD	Valerato de estradiol	12A20-N10	1
Caelo	Valerato de estradiol	10E07-N04	1
Caelo	Valerato de estradiol	12G05-N09	2
Caelo	Valerato de estradiol	13264001	1
Caelo	Valerato de estradiol	13264002	1
Caelo	Valerato de estradiol	13264003	1
Caelo	Valerato de estradiol	14E26-B02-294844	1
Caelo	Valerato de estradiol	14E26-B02-294845	1
Caelo	Valerato de estradiol	15194808	1
Caelo	Valerato de estradiol	15C10-805	1
Caelo	Valerato de estradiol	15C10-B05	2
Caelo	Valerato de estradiol	15c10-B05-305396	1
Caelo	Valerato de estradiol	15C10B05308851	1
Caelo	Valerato de estradiol	15c10-b05-314840	1
Caelo	Valerato de estradiol	15C10-B05-314840	1
Caelo	Valerato de estradiol	15C10-B05-321675	1
Caelo	Valerato de estradiol	15C10-B05-326087	1
Caelo	Valerato de estradiol	16327702	5
Caelo	Valerato de estradiol	16327703	2
Caelo	Valerato de estradiol	16327706	4
Caelo	Valerato de estradiol	16327709	5
Caelo	Valerato de estradiol	16327710	1
Caelo	Valerato de estradiol	16327711	3
Caelo	Valerato de estradiol	16F09-B01-332756	1
Caelo	Valerato de estradiol	18062402	1
Caelo	Valerato de estradiol	18067402	11
Caelo	Valerato de estradiol	18067403	1
Caelo	Valerato de estradiol	18067404	1
Caelo	Valerato de estradiol	18067405	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valerato de estradiol	18067407	8
Caelo	Valerato de estradiol	18067408	2
Caelo	Valerato de estradiol	18067409	7
Caelo	Valerato de estradiol	18067410	1
Caelo	Valerato de estradiol	18067410P-181228-1	1
Caelo	Valerato de estradiol	18067411	1
Caelo	Valerato de estradiol	18067412	3
Caelo	Valerato de estradiol	18067413	2
Caelo	Valerato de estradiol	18067415P-190718-2	1
Caelo	Valerato de estradiol	18067416	6
Caelo	Valerato de estradiol	18067417	1
Caelo	Valerato de estradiol	18067417P-200217-3	1
Caelo	Valerato de estradiol	1810013	1
Caelo	Valerato de estradiol	190615001	4
Caelo	Valerato de estradiol	190615003	1
Caelo	Valerato de estradiol	190615004	13
Caelo	Valerato de estradiol	190615007	3
Caelo	Valerato de estradiol	19061501	2
Caelo	Valerato de estradiol	19061503	4
Caelo	Valerato de estradiol	19061506	5
Caelo	Valerato de estradiol	19061507	10
Caelo	Valerato de estradiol	200004423006	1
Caelo	Valerato de estradiol	20002389002	19
Caelo	Valerato de estradiol	20002389003	11
Caelo	Valerato de estradiol	20004423001	12
Caelo	Valerato de estradiol	20004423003	5
Caelo	Valerato de estradiol	20004423005	3
Caelo	Valerato de estradiol	20004423006	9
Caelo	Valerato de estradiol	2000443001	1
Caelo	Valerato de estradiol	2002389002	1
Caelo	Valerato de estradiol	218U-03259	1
Caelo	Valerato de estradiol	22000384004	2
Caelo	Valerato de estradiol	22000384007	1
Caelo	Valerato de estradiol	4(20002389002)	1
Caelo	Valerato de estradiol	4214U-03259	1
Caelo	Valerato de estradiol	5218Q-03259	1
Caelo	Valerato de estradiol	5315A-03259	1
Caelo	Valerato de estradiol	test	1
Caesar & Lorenz	Valerato de estradiol	10123258	1
Caesar & Loretz GmbH...	Valerato de estradiol	20004423003	1
Caesar & Loretz GmbH...	Valerato de estradiol	20004423006	1
Caesar & Loretz GmbH...	Valerato de estradiol	22000384004	1
Caesar & Loretz GmbH...	Valerato de estradiol	20004423005	1
Caesar & Loretz GmbH/Gehe	Valerato de estradiol	190615	1
Caesar & Loretz GmbH/Gehe	Valerato de estradiol	190615004	1
Caesar & Loretz GmbH/Kehr	Valerato de estradiol	18067409	1
Caesar & Loretz GmbH/Kehr	Valerato de estradiol	18067416	1
Caesar & Loretz GmbH...	Valerato de estradiol	20004423005	1
Caesar & Loretz GmbH...	Valerato de estradiol	19061501	1
Caesar & Loretz GmbH...	Valerato de estradiol	19061507	4
Caesar & Loretz GmbH...	Valerato de estradiol	20004423006	3
Caesar & Loretz GmbH...	Valerato de estradiol	20002389002	1
Caesar & Loretz GmbH	Valerato de estradiol	18067416	1
Caesar & Loretz GmbH	Valerato de estradiol	18067417	1
CAESAR & LORETZ GMBH	Valerato de estradiol	190615001	1
CAESAR & LORETZ GMBH	Valerato de estradiol	190615003	2
Caesar & Loretz GmbH	Valerato de estradiol	190615004	4
Caesar & Loretz GmbH	Valerato de estradiol	19061503	2
Caesar & Loretz GmbH	Valerato de estradiol	19061507	1
Caesar & Loretz GmbH	Valerato de estradiol	20002389002	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Valerato de estradiol	20002389003	2
Caesar & Loretz GmbH	Valerato de estradiol	20004423001	5
Caesar & Loretz GmbH	Valerato de estradiol	20004423003	3
Caesar & Loretz GmbH	Valerato de estradiol	20004423006	7
Caesar & Loretz GmbH	Valerato de estradiol	22000384002	4
Caesar & Loretz GmbH	Valerato de estradiol	22000384004	4
Caesar & Loretz GmbH	Valerato de estradiol	22000384005	1
Cealo/Sanacorp	Valerato de estradiol	20004423006	1
Euro OTC	Valerato de estradiol	15C10-b05	1
Euro OTC	Valerato de estradiol	1606022-01	1
Faegon	Valerato de estradiol	15C10-B05-324956	2
Fagro	Valerato de estradiol	15C10-B05-318405	1
Fagron	Valerato de estradiol	11G18-N04	1
Fagron	Valerato de estradiol	11J13-N09	1
Fagron	Valerato de estradiol	11J13-No9	1
Fagron	Valerato de estradiol	11k04-n04	1
Fagron	Valerato de estradiol	11K04-N04	1
Fagron	Valerato de estradiol	12A20-N10	2
Fagron	Valerato de estradiol	12D18-N02	3
Fagron	Valerato de estradiol	12G05N09	1
Fagron	Valerato de estradiol	12G05-N09	2
Fagron	Valerato de estradiol	12K05-N02	3
Fagron	Valerato de estradiol	13A07-N11	6
Fagron	Valerato de estradiol	13D16N10	1
Fagron	Valerato de estradiol	13D16-N10	4
Fagron	Valerato de estradiol	13g09-n05	1
Fagron	Valerato de estradiol	13G09N05	1
Fagron	Valerato de estradiol	13G09-N05	5
Fagron	Valerato de estradiol	13I13-N02	2
Fagron	Valerato de estradiol	13J13-N02	1
Fagron	Valerato de estradiol	14E26B02	2
Fagron	Valerato de estradiol	14E26-B02-294844	1
Fagron	Valerato de estradiol	14E26-B02-294845	3
Fagron	Valerato de estradiol	14E26-B02-294847	1
Fagron	Valerato de estradiol	14E26-B02-296348	7
Fagron	Valerato de estradiol	14E26-B02-302873	3
Fagron	Valerato de estradiol	15C10-B05	2
Fagron	Valerato de estradiol	15C10-B05_314840	1
Fagron	Valerato de estradiol	15C10-B05-305395	6
Fagron	Valerato de estradiol	15C10-B05-305396	1
Fagron	Valerato de estradiol	15C10-B05-308851	9
Fagron	Valerato de estradiol	15c10-b05-309186	1
Fagron	Valerato de estradiol	15C10-B05-309186	3
Fagron	Valerato de estradiol	15C10-B05-313568	1
Fagron	Valerato de estradiol	15c10-b05-314840	1
Fagron	Valerato de estradiol	15C10-B05-314840	5
Fagron	Valerato de estradiol	15C10-B05-318405	1
Fagron	Valerato de estradiol	15C10B05321675	1
Fagron	Valerato de estradiol	15C10-B05-321675	11
Fagron	Valerato de estradiol	15c10-b05-324956	1
Fagron	Valerato de estradiol	15C10-B05-324956	1
Fagron	Valerato de estradiol	15C10B05-326087	1
Fagron	Valerato de estradiol	15C10-B05-326087	5
Fagron	Valerato de estradiol	16F09-B01	2
Fagron	Valerato de estradiol	16F09-B01_332756	1
Fagron	Valerato de estradiol	16F09-B01-328135	8
Fagron	Valerato de estradiol	16F09-B01-329621	1
Fagron	Valerato de estradiol	16F09-B01-332756	5
Fagron	Valerato de estradiol	16F09-B01-332757	2
Fagron	Valerato de estradiol	16F09Bo1328135	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Valerato de estradiol	18067405	1
Fagron	Valerato de estradiol	18g05-b02	1
Fagron	Valerato de estradiol	18G05-B02	2
Fagron	Valerato de estradiol	18G05-B02-353985	13
Fagron	Valerato de estradiol	18G05-B02353986	1
Fagron	Valerato de estradiol	18G05-B02-353986	3
Fagron	Valerato de estradiol	18G5-B02-253985	1
Fagron	Valerato de estradiol	190615001	1
Fagron	Valerato de estradiol	19c10-b05-318405	1
Fagron	Valerato de estradiol	20002389003	1
Fagron	Valerato de estradiol	20J16-F01	2
Fagron	Valerato de estradiol	20J16-F01-3760807	1
Fagron	Valerato de estradiol	20J16F01376087	2
Fagron	Valerato de estradiol	20J16-F01-376087	3
Fagron	Valerato de estradiol	23A30-B05-224547	1
Fagron	Valerato de estradiol	24052014a	1
Fagron	Valerato de estradiol	27061710	1
Fagron	Valerato de estradiol	814M-03259	1
Fagron	Valerato de estradiol	82201620	1
Fagron	Valerato de estradiol	84404140	4
Fagron	Valerato de estradiol	ESV003-1A	2
Fagron	Valerato de estradiol	ESVOO3-1A	1
Fagron	Valerato de estradiol	F01-3751904	1
Fagron	Valerato de estradiol	VFM002-1C	2
Fargon / AHD	Valerato de estradiol	18G05-B02-353985	2
fargon/Phoenix	Valerato de estradiol	16F09-B01-332756	2
Fargon	Valerato de estradiol	10123264	1
Frago/Gehe	Valerato de estradiol	15C10-B0508561040	1
Frago/Noweda	Valerato de estradiol	16F09-B01	2
Frago/Noweda	Valerato de estradiol	16F09-B01-329621	1
Frago/Noweda	Valerato de estradiol	16F09-B01-332757	1
Fragon	Valerato de estradiol	15C10-B05-5314840	1
Gehe	Valerato de estradiol	14E26-B02-296348	1
Gehe	Valerato de estradiol	14E26-B02-302872	1
Gehe	Valerato de estradiol	16327703	1
Gehe	Valerato de estradiol	16327712	1
Gehe	Valerato de estradiol	16F09-B01-332756	1
GEHE	Valerato de estradiol	16F09-B01-332757	1
Gehe	Valerato de estradiol	190615001	1
Hedinger/Noweda	Valerato de estradiol	15C10-B05	1
Noweda	Valerato de estradiol	12A20-N10	1
Noweda	Valerato de estradiol	19061506	1
Noweda	Valerato de estradiol	20002389003	1
noweda	Valerato de estradiol	2200034007	1
Noweda	Valerato de estradiol	22000384015	1
Phoenix	Valerato de estradiol	13G09-N05	1
Phoenix	Valerato de estradiol	20002389002	1
Phoenix	Valerato de estradiol	20J16-F01-375194	1
Phönix/Fargon	Valerato de estradiol	979-32-8	1
Phönix	Valerato de estradiol	15C10-B05-326087	1
phönix	Valerato de estradiol	20J16-F01	1
Röntgen	Valerato de estradiol	190615004	2
Sanacorp	Valerato de estradiol	13264002	1
Sanacorp	Valerato de estradiol	20J16-F01-375194	1
Sanacorp	Valerato de estradiol	22000384015	1
THC/Phönix	Valerato de estradiol	18067402	1

- 235 567 spectra from 1515 *Apo-Ident* customers from a total of 49 113 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Valerato de estradiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Valerato de estradiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	820	0	152 142
Type B	0	467	0	201 617
Type C	0	492	8	235 567

The substance/substance group *Valerato de estradiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2683 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7152 %)
Type C	100.0000 % (> 99.9007 %)	98.4000 % (> 97.8000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20651	21411	5,63	126,35
21266	21416	6,29	128,75
21411	21411	0,00	125,50
21416	21416	0,00	128,51
21417	21416	2,65	129,03
21418	21416	4,99	126,77
21419	21416	1,87	128,95
21422	21416	3,72	129,47
21423	21416	3,00	127,83
21424	21424	0,00	128,94
21425	21416	2,39	129,60
21426	21416	1,88	129,03

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21646	21416	5,49	129,26
21989	21416	2,72	129,89
23056	23056	0,00	128,64
26741	21416	10,35	127,44

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Valina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20405-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Valina; Valinum

Special notes

When selecting the *Valina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Valina	7	13	14

Second-stage model

For differentiation of the substance/substance group *Valina* the following second-stage model is used:

- Submodelo 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Valina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Isoleucina	66,13	–
⋮	⋮	⋮
Levocarnitina	>50	36,45
Cloridrato de oxibutinina	>50	118,88
Acetato de ciproterona	>50	155,24
Prednicarbato	>50	174,37
Capsaicina	>50	188,18
Citrato de sódio	>50	225,46
Cloridrato de amitriptilina	>50	319,49
Acetato de noretisterona	>50	355,15
Tetracaína	>50	365,76
Metoxisaleno	>50	367,34
Piridoxal-5-fosfato	>50	398,82
Alfaestradiol	>50	467,93
Cloridrato de quinina di-hidratado	>50	546,36
Cloridrato de ciprofloxacina	>50	646,78
Heparina sódica	>50	813,07
Triclosan	>50	1728,14
Amifampridina	>50	2472,77
Sacarose	>50	2528,31

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Valina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Valina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Valina	1604055	22571	40	20160601*
Euro OTC	Valina	1701026	23131	40	20170222*
Euro OTC	Valina	1904006	24611	40	20190423*
Euro OTC	Valina	1909028	24971	40	20191015*
Euro OTC	Valina	2004021	25169	40	20200505*
Euro OTC	Valina	2006020	25335	40	20200814*
Fagron	Valina	15A14-B07-307756	21953	60	9198

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Valina*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 662 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 570 spectra of 16 reference samples from the substance/substance group *Valina*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Valina	1609009	22799	40
Euro OTC	Valina	1705017	23426	40
Euro OTC	Valina	1710003	23770	40
Euro OTC	Valina	1712005	23867	40
Euro OTC	Valina	1803017	24091	40
Euro OTC	Valina	1805014	24119	40
Euro OTC	Valina	1809027	24304	40
Euro OTC	Valina	2009046	25422	40
Euro OTC	Valina	2201022	25962	40
Euro OTC	Valina	2205007	26190	40
Euro OTC	Valina	2301008	26574	40
Euro OTC	Valina	2308006	26880	40
Euro OTC	Valina	2403016	27282	40
Euro OTC	Valina	2201022	25962SI	10
Euro OTC	Valina	2205007	26190SI	20
Euro OTC	Valina	2301008	26574SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 514 spectra from a total of 4032 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 10 *Apo-Ident* customers from 14 batches from the substance/substance group *Valina*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Valina	2006020-01	3
Euro OTC	Valina	1604055-01	2
Euro OTC	Valina	1710003-01	1
Euro OTC	Valina	1805014-01	1
Euro OTC	Valina	1805014-02	2
Euro OTC	Valina	2009045-03	1
Euro OTC	Valina	2009046-01	2
Euro OTC	Valina	2009046-03	1
Euro OTC	Valina	L1309029-02	1
Fagron	Valina	121259	1
Fagron	Valina	13B13-N05	1
Fagron	Valina	17B27-B03-336205	1
Fagron	Valina	17H14-B04	1
Fagron	Valina	20B12-B02-196844	1

- 236 048 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Valina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Valina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	570	0	201 514
Type C	0	18	1	236 048

The substance/substance group *Valina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9474 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21953	21953	0,00	99,70
22571	22571	0,00	99,97
23131	23131	0,00	100,82
24611	24611	0,00	97,52
24971	24971	0,00	98,79
25169	25169	0,00	103,69
25335	25335	0,00	102,01

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Vanilina**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20204-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Vanilina; Vanillinum

Special notes

When selecting the *Vanilina* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Vanilina	6	4	60

Second-stage model

For differentiation of the substance/substance group *Vanilina* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Vanilina* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cromoglicato de sódio	98,90	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Vanilina* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Vanilina*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Vanilina	14044413	21737	60	20140227
Caelo	Vanilina	15135302	21924	60	AR-17-FG-022168-03
Caelo	Vanilina	160895	22484	60	20160421*
Caelo	Vanilina	191201	24719	40	20190515*
Caelo	Vanilina	22001135	26109	40	20220408*
Fagron	Vanilina	13J01-N07	21738	60	20130926

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 6 reference samples from the substance/substance group *Vanilina*. These samples

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Vanilina*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Vanilina	171172	23308	40
Caelo	Vanilina	17117201	23561	40
Caelo	Vanilina	173088	23805	40
Caelo	Vanilina	23003197	27118	40
Caelo	Vanilina	22001135	26109SI†	20
Caelo	Vanilina	23003197	27118SI	20

- 201 884 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 233 spectra from 179 *Apo-Ident* customers from 64 batches from the substance/substance group *Vanilina*.
- Among them are spectra of independent samples from 60 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Vanilina	21001092003	1
	Vanilina	22001135004	4
	Vanilina	22001135012	1
	Vanilina	23003197003	1
Anzag	Vanilina	12H09-N06	1
Anzag	Vanilina	16089508	1
Caelo	Vanilina		1
Caelo	Vanilina	10066811	1
Caelo	Vanilina	10066830	1
Caelo	Vanilina	1089501	1
Caelo	Vanilina	112901	1
Caelo	Vanilina	12071401	1
Caelo	Vanilina	12079407	2
Caelo	Vanilina	12079410	2
Caelo	Vanilina	12079412	2
Caelo	Vanilina	12079417	1
Caelo	Vanilina	12079424	2
Caelo	Vanilina	12079428	1
Caelo	Vanilina	14044419	3
Caelo	Vanilina	15135302	2
Caelo	Vanilina	1514006	1
Caelo	Vanilina	15154006	1
Caelo	Vanilina	15154014	4
Caelo	Vanilina	15154017	2
Caelo	Vanilina	15154020	6
Caelo	Vanilina	15227317	1
Caelo	Vanilina	16089501	3
Caelo	Vanilina	16089506	12
Caelo	Vanilina	16089508	3
Caelo	Vanilina	17117201	2
Caelo	Vanilina	17117207	19
Caelo	Vanilina	17117208	3
Caelo	Vanilina	18073501	9
Caelo	Vanilina	18073506	3
Caelo	Vanilina	18073507	7
Caelo	Vanilina	18073509	4
Caelo	Vanilina	18073511	5
Caelo	Vanilina	18073515	5
Caelo	Vanilina	191201005	9
Caelo	Vanilina	19120102	9
Caelo	Vanilina	20000477003	4
Caelo	Vanilina	20003608002	4
Caelo	Vanilina	20003608006	4
Caelo	Vanilina	2000477003	1
Caelo	Vanilina	21001092003	5
Caelo	Vanilina	21001092009	5
Caelo	Vanilina	211029	1
Caelo	Vanilina	2200135004	2
Caelo	Vanilina	250220004773	1
Caelo	Vanilina	4216I-02548	1
Caelo	Vanilina	90961269	1
Caesar & Loretz GmbH...	Vanilina	21001092003	1
Caesar & Loretz GmbH...	Vanilina	18073515	1
Caesar & Loretz GmbH...	Vanilina	18073507	1
Caesar & Loretz GmbH...	Vanilina	10066830	1
Caesar & Loretz GmbH...	Vanilina	12079401	1
Caesar & Loretz GmbH...	Vanilina	12079412	1
Caesar & Loretz GmbH	Vanilina	18073511	1
Caesar & Loretz GmbH	Vanilina	18073515	1
Caesar & Loretz GmbH	Vanilina	191201005	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Vanilina	20000477003	1
Caesar & Loretz GmbH	Vanilina	20003608002	3
Caesar & Loretz GmbH	Vanilina	20003608006	1
Caesar & Loretz GmbH	Vanilina	21001092003	2
Caesar & Loretz GmbH	Vanilina	21001092009	4
Caesar & Loretz GmbH	Vanilina	22001135011	1
Caesar & Loretz/Geil...	Vanilina	191201005	1
Caleo / Phoenix	Vanilina	20000477003	1
Dr.Hollborn	Vanilina	6082015	1
Fagron	Vanilina	11G28-N09	1
Fagron	Vanilina	12D02-N03	1
Fagron	Vanilina	12H09-N06	2
Fagron	Vanilina	13J01-N07	6
Fagron	Vanilina	14G02-B99-296988	1
Fagron	Vanilina	18073501	1
Fagron	Vanilina	232050-0004	1
Fagron	Vanilina	314Q2548	1
Fagron	Vanilina	8L05-N07	1
fargron	Vanilina	13/01-N07	1
Finteler Apotheke	Vanilina	17117201	1
Gatt-Koller	Vanilina	201770800	1
Gehe/Noweda	Vanilina	15154006	1
Gehe	Vanilina	12079412	1
Gehe	Vanilina	16089506	1
Gehe	Vanilina	20000477003	1
Hedinger/Ebert	Vanilina	13A30-N10	1
Jenne	Vanilina	18073501	1
Klosterring	Vanilina	17117207	1
L10	Vanilina	18073506	1
L12	Vanilina	16089508	1
L12	Vanilina	17117201	1
L12	Vanilina	18073501	1
labor	Vanilina	101010101	1
Noweda	Vanilina	18073501	1
Phoenix	Vanilina	21001092003	1
Reagenz Ph.Eur.	Vanilina		1
Rhodia GmbH/Noweda	Vanilina	12D02-N03	1
Sanacorp	Vanilina	12H09-N06	1
Sanacorp	Vanilina	20000477003	1

- 235 834 spectra from 1515 *Apo-Ident* customers from a total of 49 197 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Vanilina* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Vanilina* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	200	0	201 884
Type C	0	232	1	235 834

The substance/substance group *Vanilina* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.5708 % (> 98.2833 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21737	21924	2,90	197,24
21738	21924	3,96	201,46
21924	21924	0,00	189,07
22484	22484	0,00	205,79
24719	24719	0,00	208,48
26109	26109	0,00	221,14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Xilitol**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20994-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xilitol; Xylitolum

Special notes

When selecting the *Xilitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Xilitol	7	5	24

Second-stage model

For differentiation of the substance/substance group *Xilitol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Xilitol* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	70,16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Xilitol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xilitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xilitol	14068206	21755	60	20140317
Caelo	Xilitol	15135405	22248	60	20150417
Caelo	Xilitol	15135405	22579	40	20150417
Caelo	Xilitol	20002926	25619	40	20201027*
Caelo	Xilitol	23000539	26692	40	20230331*
Caelo	Xilitol	23000539	26692SI	20	20230331*
Caelo	Xilitol	24000699	27256	40	20240411*
Caelo	Xilitol	24000699	27256SI	20	20240411*
Fagron	Xilitol	14G04-B04-298356	21754	60	AR-15-FG-008046-01
Fagron	Xilitol	14G04-B04-303524	22254	60	20140919

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Xilitol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

batches.

- 152 522 spectra from a total of 2835 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 6 reference samples from the substance/substance group *Xilitol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xilitol	15388101	22578	40
Caelo	Xilitol	163174	23061	40
Caelo	Xilitol	181133	24041	40
Caelo	Xilitol	21004147	26002	40
Caelo	Xilitol	24002073	27306	40
Caelo	Xilitol	21004147	26002SI	10

- 201 874 spectra from a total of 4040 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 40 spectra from 19 *Apo-Ident* customers from 27 batches from the substance/substance group *Xilitol*.

- Among them are spectra of independent samples from 24 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Xilitol	23000699002	1
Caelo	Xilitol	1219Q-02787	1
Caelo	Xilitol	12240612	1
Caelo	Xilitol	13230302	1
Caelo	Xilitol	13230305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Xilitol	13230309	1
Caelo	Xilitol	13230315	1
Caelo	Xilitol	14061401	1
Caelo	Xilitol	14068206	1
Caelo	Xilitol	14G04-B04-298356	2
Caelo	Xilitol	15388104	3
Caelo	Xilitol	16317401	1
Caelo	Xilitol	18045302	4
Caelo	Xilitol	18113304	1
Caelo	Xilitol	18235908	1
Caelo	Xilitol	19120404	2
Caelo	Xilitol	20003607001	2
Caelo	Xilitol	3314M-02787	1
Caelo	Xilitol	5112I-02787	1
Caelo	Xilitol	718I-02787	1
Caesar & Loretz GmbH	Xilitol	20003607001	2
Caesar & Loretz GmbH	Xilitol	20003607013	1
Fagron	Xilitol	12J25-N06	2
Fagron	Xilitol	13/23-N06	1
Fagron	Xilitol	13H28N10	1
Fagron	Xilitol	13H28-N10	2
Fagron	Xilitol	14G04-B04-303524	2
Fagron	Xilitol	16c14-B02-320887	1

- 236 027 spectra from 1515 *Apo-Ident* customers from a total of 49 231 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xilitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xilitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	210	0	201 874
Type C	0	40	0	236 027

The substance/substance group *Xilitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 85.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21754	21754	0,00	187,37
21755	26692	6,79	182,74
22248	26692	6,20	182,56
22254	21754	5,48	184,62
22579	27256	6,90	185,07
25619	25619	0,00	183,26
26692	26692	0,00	182,03
27256	27256	0,00	185,29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Xilose**
Substance class	BR IFAs e excipientes sólidos
Report date	07/03/2025
Report number	20517-2025-03-07
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xilose; Xylosum

Special notes

When selecting the *Xilose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Xilose	6	7	27

Second-stage model

For differentiation of the substance/substance group *Xilose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Xilose* in the substance class *BR IFAs e excipientes sólidos*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sulfato de polimixina B	81,21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Xilose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xilose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xilose	14218902	21606	60	AR-14-FG-013086-01
Caelo	Xilose	17160902	23413	40	20170704
Caelo	Xilose	191802002	25437	40	20190819
Caelo	Xilose	21000133001	25732	50	20210219
Fagron	Xilose	13A31-B40-292395	21763	60	20140407
Fagron	Xilose	16A25-B05-328261	23524	40	20160215

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 290 spectra of 6 reference samples from the substance/substance group *Xilose*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 672 spectra from a total of 2836 batches from further 485 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 9 reference samples from the substance/substance group *Xilose*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xilose	13133402	20868	40
Caelo	Xilose	162064	22758	40
Caelo	Xilose	171609	23656	40
Caelo	Xilose	173188	23849	40
Caelo	Xilose	190499	24527	40
Caelo	Xilose	22000045004	26310	30
Caelo	Xilose	23000619	27123	40
Caelo	Xilose	22000045004	26310SI	20
Caelo	Xilose	23000619	27123SI	20

- 201 774 spectra from a total of 4038 batches from further 842 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 45 spectra from 15 *Apo-Ident* customers from 29 batches from the substance/substance group *Xilose*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Xilose	23000619001	2
Caelo	Xilose	11031501	1
Caelo	Xilose	12120101	1
Caelo	Xilose	13133404	2
Caelo	Xilose	13133410	1
Caelo	Xilose	13133414	3
Caelo	Xilose	16002301	3
Caelo	Xilose	16002302	2
Caelo	Xilose	16002309	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Xilose	16206405	1
Caelo	Xilose	17160902	2
Caelo	Xilose	17160905	2
Caelo	Xilose	17318803	4
Caelo	Xilose	17318809	1
Caelo	Xilose	19049902	1
Caelo	Xilose	19180205	2
Caelo	Xilose	21000133002	1
Caelo	Xilose	5031501	1
Caesar & Loretz GmbH	Xilose	20000783003	2
Eigenherstellung	Xilose	80414HJK01	1
Euro OTC	Xilose		1
Fagron	Xilose	10121401	1
Fagron	Xilose	13133415	1
Fagron	Xilose	14E-B03_300658	1
Fagron	Xilose	28111405	1
Fagron	Xilose	80414PJK01	1
Falcento	Xilose	2013051801	1
Phoenix 20.06.2014	Xilose	13A31-B04-292396	1
Phoenix Goettin	Xilose	13133422	1

- 236 022 spectra from 1515 *Apo-Ident* customers from a total of 49 229 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xilose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xilose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	310	0	201 774
Type C	0	45	0	236 022

The substance/substance group *Xilose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.6667 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21606	21606	0,00	155,42
21763	21606	21,01	156,70
23413	21606	17,27	157,75
23524	21606	18,77	154,33
25437	21606	27,27	176,50
25732	21606	18,50	168,18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

Appendix A: Additional calibration samples (*Type A*)

Substance spectra also enter the generation of the chemometric model which cannot be identified with this model. This serves the purpose that substances which the model is not supposed to recognise are safely rejected. The spectra of these samples are entered into the validation as *Type A*. They were recorded by *HiperScan GmbH*.

The samples originate from 162 batches. From these, 6750 spectra were recorded. The calibration spectra of substances which can be identified with the model are listed respectively in the section *calibration samples* for the individual substances and do not appear again elsewhere in this list.

Supplier	Substance	Batch	Spectra	Certificate
Sigma-Aldrich	Acetato de betametasona	LRAA8500	40	CRS
Fagron	Acetato de mafenida	20K06-B04-211072	40	20201229
Fagron	Acetato de mafenida	22B02-B03-222844	40	241107539
Euro OTC	Ácido desoxicólico	1305051-01	40	from supplier
New Zealan…	Ácido desoxicólico	0416720	40	from supplier
Safic-Alcan	Ácido dimercaptossuccínico	20170210	40	from supplier
Flora Apot…	Ácido glicirrízico	10588	40	from supplier
Caelo	Alcarávia	11003217	40	20110209
Caelo	Aloés, cabo	11048808	40	20110315
Fagron	Amarelo crepúsculo S	13I05_N04	40	20130903
Flora Apot…	Amigdalina	13121802	40	1405619
Auropure L…	Amigdalina, extrato de amêndoa amarga 98%	PA02099-17102131	40	from supplier
Safic-Alcan	Amigdalina, extrato de amêndoa amarga 98%	BAE150902	60	from supplier
Safic-Alcan	Amigdalina, extrato de amêndoa amarga 98%	BAE150902	60	from supplier
Caelo	Anis	13333903	40	20131018
Caelo	Anis estrelado	11314104	30	20111121
Caelo	Anis, esmagado	13357101	40	20131202
Caelo	Babosa da montanha, pulverizada	12183008	40	20120802
Caelo	Bagas de zimbro, esmagado	13367302	40	20131122
Euro OTC	Benfotiamina	2207006	40	20220729*
Euro OTC	Benfotiamina	2207006	20	20220729*
Caelo	Benjoim do Sião (Styrax tonkinensis)	12321312	40	pending
Caelo	Benjoim do Sião (Styrax tonkinensis)	12321314	40	20121031
Fagron	Butirato de hidrocortisona	15J12-B03-322394	40	20151028
Euro OTC	Carbonato de cálcio	1611008-01	40	20161201
Caelo	Carbonato de magnésio, pesado	182282	40	20180906*
Klenk	Casca de bétula, cortada	0561A121121	40	20121127
Caelo	Castoreum pulverizado	12137409	40	1402590
Caelo	Cera de carnaúba	170903	40	20170512*
Caelo	Cera de carnaúba	183330	40	20190114*
Caelo	Chicória, raiz (Cichorium intybus)	11374504	40	20120112
Caelo	Cloreto de benzalcônio	16171603	40	20160715
Caelo	Cloridrato de buprenorfina	12172908	40	0814I-07774
Caelo	Cloridrato de buprenorfina	16143001	40	2017A-07774
Euro OTC	Cloridrato de fexofenadina	2310018	30	20240222*
Dr. Behr	Cloridrato de L-carnitina	WE11030091	60	from supplier
Flora Apot…	Cloridrato de levamisol	LV17203	40	from supplier
Caelo	Colofônia	12301410	60	AR-15-FG-016314-01
Caelo	Colofônia	173014	40	20180102*
Caelo	Colofônia	191664	40	20190701*
Klenk	Cominho pulverizado	2824B121001	40	20121009

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Euro OTC	Concentrado seco de colecalciferol	1508032	60	20150901*
Euro OTC	Concentrado seco de colecalciferol	1608002	40	20160824*
Euro OTC	Concentrado seco de colecalciferol	2001007	40	20200316*
Klenk	Cravo pulverizado (especiaria)	1264B141007	60	AR-15-FG-014858-01
Sigma-Aldrich	Diclofenaco potássico	D1039990	40	CRS
Pharmorgana	Dicloroacetato de sódio	1000150016	40	from supplier
Caelo	Endro, cortado	11295103	40	20111103
Yino Pharma	Enoxaparina sódica	YN010232209001	40	20230524*
Yino Pharma	Enoxaparina sódica	YN010232210002	40	20230524*
Yino Pharma	Enoxaparina sódica	YN010232209001	20	20230524*
Yino Pharma	Enoxaparina sódica	YN010232210002	20	20230524*
Bombastus	Estróbilo de lúpulo	23003461	30	20230809
Euro OTC	Extrato de semente de Griffonia	1205027	40	from supplier
Euro OTC	Extrato de semente de Griffonia	1705007	40	20170601*
Euro OTC	Extrato de semente de Griffonia	1905017	40	20190709*
Pharmorgana	Extrato de semente de Griffonia	1000200297	40	from supplier
Caelo	Feijão, cascas	11030601	50	20110221
Klenk	Flor de calêndula	1241B130321	40	20130408
Caelo	Flor de calêndula, cortada	11187605	40	20110930
Caelo	Flor de camomila-vulgar	12337605	40	20121122
Caelo	Folha de alecrim	11193408	40	20110728
Caelo	Folha de erva-cidreira	13214713	40	20130806
Caelo	Folha de eucalipto	11307706	40	20111111
Caelo	Folha de hortelã-pimenta	11347607	40	20111220
Flora Apot...	Fosfato de colamina de cálcio	14384	40	from supplier
Pharmorgana	Fosfato de colamina de cálcio	1000200822	40	from supplier
Pharmorgana	Fosfato de colamina de cálcio	1000210678	50	from supplier
Pharmorgana	Fosfato de colamina de cálcio	1000230793	40	from supplier
Th. Geyer	Fosfato de colamina de cálcio	33299	60	from supplier
Th. Geyer	Fosfato de colamina de cálcio	66606	40	from supplier
Flora Apot...	Fosfato de Mg-Ca-K-colamina	1000190952	40	from supplier
Th. Geyer	Fosfato de Mg-Ca-K-colamina	36985	60	from supplier
Th. Geyer	Fosfato de Mg-Ca-K-colamina	46816	40	from supplier
Th. Geyer	Fosfato de Mg-Ca-K-colamina	80919	40	from supplier
Sigma-Aldrich	Fosfato dissódico de betametasona	MKBS9676V	40	CRS
Sigma-Aldrich	Fosfato dissódico de dexametasona	LRAC1690	40	CRS
Caelo	Fruto da alcarávia, esmagada	12116904	40	20120503
Klenk	Fruto do aipo	7140A131122	60	20131204
Caelo	Gengibre	12180601	40	20120730

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Gengibre	11325715	40	20111205
Klenk	Gengibre, descascado, pulverizado	6954B160429	60	1704440
Caelo	Groselha	12272801	40	1403468
EDQM	Hexacetonida de triancinolona	3.0	40	CRS
Fagron	Ivermectina	23L22-H07-00747	40	20231228
Fagron	Ivermectina	23L22-H07-00747	20	20231228
FSA Chemicals	Ivermectina	23J18-AP24014	40	241107538
Euro OTC	Kaliumorotat	1203038V-02	60	from supplier
Euro OTC	Kaliumorotat	1203038V-02	40	9757
Flora Apot...	Kaliumorotat	ORK00117	40	from supplier
Caelo	Kelp, cortado	13230805	40	AR-15-FG-007678-01
Caelo	Kelp, cortado	15418801	60	AR-17-FG-007505-01
Fagron	L-5-hidroxitriptofano	22A17-B03-226102	40	240603342
EDQM	Lactobionato de eritromicina	1.0	40	CRS
Pharmorgana	L-aspartato de cálcio trihidratado	1000230427	40	from supplier
Caelo	Linhaça	12186902	60	pending
Caelo	Linhaça	13412801	40	20140113
Fagron	Losartana potássica	D5440-24-006	40	20240410*
Caelo	Melilotus vulgaris	12317104	40	20121122
Klenk	Melilotus vulgaris	1400A130304	40	20130403
Caelo	Mirra	11277111	60	1403081
Caelo	Mirra	13108701	40	AR-15-FG-000946-01
Caelo	Mirtilo seco	10265602	40	20101206
Caelo	Musgo-da Islândia	12187106	40	1403493
Caelo	Musgo-da Islândia	13350803	40	20131114
Fagron	Nitrato de econazol	12H08-N02	40	1312442
Fagron	Nitrato de econazol	11F09-N16	40	20110606
Fagron	Nitrato de econazol	12I06-B40-306925	40	AR-16-FG-011359-01
Fagron	Nitrato de econazol	14G22-B07-327805	40	20140804
EDQM	Nitrato de fenticonazol	1.3	40	CRS
Klenk	Noz-moscada, pulverizada (especiaria)	7325A160405	60	9888
Flora Apot...	Olíbano	JR-RX20230716CG	40	not required
Euro OTC	Orotato de cálcio dihidratado	1401006-01	40	1412540
Euro OTC	Orotato de cálcio dihidratado	1603003	40	20160329*
Euro OTC	Orotato de cálcio dihidratado	1603003	40	20180615*
Fagron	Orotato de cálcio dihidratado	12L04-N07	40	from supplier
Fagron	Orotato de cálcio dihidratado	13J23-N05	40	from supplier
Flora Apot...	Orotato de cálcio dihidratado	ORC00119	40	from supplier
Pharmorgana	Orotato de cromo (III) hexahidratado	760020	40	from supplier
Merck KGaA	Peróxido de benzoíla, hidratado	S7012241509	60	20130317
Caelo	Pimenta	11193905	40	20110727
Caelo	Psyllium, cascas	13238005	40	20130816
Fagron	Pullulan	24H27-B078	40	20240916*
Klenk	Raiz de aipo, cortada	6091A110110	40	1410177
Galke	Raiz de alcaçuz, descascada	22728	40	from supplier
Klenk	Raiz de aspargo, cortada	6151B110304	40	1403480
Klenk	Raiz de confrei	6244B130624	40	20130625

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Raiz de marshmallow	11101905	40	20110406
Caelo	Raiz de marshmallow	13214804	40	20130806
Caelo	Raiz de Orris	11026705	40	20110221
Caelo	Ruibarbo	11057818	40	20110314
Caelo	Semente de cominho preto	161157	60	20160708
Caelo	Semente de mostarda preta, pulverizada	12350204	80	1403711
Caelo	Semente de mostarda, branca, pulverizada	12349601	60	1403281
Caelo	Semente de mostarda, branca, pulverizada	12375705	40	20130110
Klenk	Semente de mostarda, preta	7430A120813	40	AR-15-FG-001050-01
Klenk	Semente de salsa	7370A130909	40	1407600
Caelo	Sinapis alba, semente	12361002	40	1403473
Caelo	Sulfato de alumínio e potássio	12144605	40	from supplier
Fagron	SyrSpend® SF Alka	17D11-B04-332593	40	20170505
Fagron	SyrSpend® SF Alka	17D11-B04-332593	40	20170505
Fagron	SyrSpend® SF Alka	17F14-B02-335945	20	1804106
Fagron	SyrSpend® SF Alka	18B21-B08-347192	40	1809264
Fagron	SyrSpend® SF Alka	18C13-B11-350851	40	20180502
Fagron	SyrSpend® SF Alka	20B25-F06-369913	40	20200424
Fagron	SyrSpend® SF Alka	23B16-F01-384773	40	20230502
Fagron	SyrSpend® SF pH4	15A26-B04-311720	40	1608352
Fagron	SyrSpend® SF pH4	15A26-B04-311720	40	20150223
Fagron	SyrSpend® SF pH4	15A26-B04-305667	40	1701055
Fagron	SyrSpend® SF pH4	19L05-F10-368874	40	20200320
Fagron	SyrSpend® SF pH4	22L20-F03-384076	40	20230124
Fagron	SyrSpend® SF pH4	23H11-F02-385247	40	20231005
Fagron	SyrSpend® SF pH4	23E23-F05-385178	40	20230807
Fagron	SyrSpend® SF pH4	22L20-F03-384076	20	20230124
Fagron	SyrSpend® SF pH4 neo	21G23-F02-379002	50	2112411
Fagron	SyrSpend® SF pH4 neo	23A18-H15-00941	40	20230120
Fagron	SyrSpend® SF pH4 neo	23C21-H01-00941	40	20230328
Fagron	SyrSpend® SF pH4 neo	23K02-H08-00941	40	20231113
Fagron	SyrSpend® SF pH4 neo	24B28-H08-00941	40	20240308
Fagron	SyrSpend® SF pH4 neo	23C21-H01-00941	20	20230328
Klenk	Tormentilha	6911B141114	60	AR-15-FG-014020-01
Caelo	Visco	11294003	30	20111027

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Appendix B: Additional validation samples (*Type B*)

It is necessary that spectra also enter the validation which cannot be identified with this model. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 1167 batches. From these 46 911 spectra were recorded. The spectra recorded on independent samples of substances which can be identified with the model are listed respectively in the section *Type B* for the individual substances and do not appear again elsewhere in this list.

Supplier	Substance	Batch	Spectra	Certificate
Fagron	5-Fluorouracila	13F19-N03	40	1402308
Fagron	5-Fluorouracila	13F19-N03	60	1608169
Fagron	5-Fluorouracila	16D01-U05/3-327376	40	20161117
Caelo	Absinto (Artemisia absinthium)	12355801	40	20121211
Klenk	Açafrão (Crocus sativus)	0384A121022	40	20121114
Caelo	Açafrão de java (Curcuma xanthorrhiza)	12185605	40	1403465
Caelo	Açafrão de java (Curcuma xanthorrhiza)	12319206	40	20121130
Caelo	Açafrão de java (Curcuma xanthorrhiza)	13262904	40	20130926
EDQM	Acetato de cortisona	6.0	20	CRS
Fagron	Acetato de mafenida	15J20-B05-342526	40	20151221
Fagron	Acetato de mafenida	20K06-B04-211072	10	20201229
Fagron	Acetato de mafenida	22B02-B03-222844	20	241107539
EDQM	Acetato de medroxiprogesterona	3.0	40	CRS
EDQM	Acetato de metilprednisolona	2.0	20	CRS
Euro OTC	Acetato de vitamina A	2303019	40	20230414*
Euro OTC	Acetato de vitamina A	2303019	20	20230414*
Fagron	Acetil-L-carnitina cloridrato	24H27-B070	40	20240923*
Fagron	Acetil-L-carnitina cloridrato	24H27-B070	20	20240923*
HiperScan	Ácido canabidiólico	19802	30	20240730
Fagron	Ácido desoxicólico	14A02-B32-303429	60	AR-16-FG-004648-01
Fagron	Ácido desoxicólico	14A02-B32-303429	40	from supplier
abcr GmbH	Ácido dimercaptossuccínico	1005874	39	from supplier
Safic-Alcan	Ácido dimercaptossuccínico	20180130	40	from supplier
Fagron	Ácido Gama-aminobutírico	1524040601	40	20240406*
Fagron	Ácido Gama-aminobutírico	1524040601	20	20240406*
abcr GmbH	Ácido glicirrízico	1222024	40	from supplier
Fagron	Ácido L-málico	15J09-B03-313987	60	9346
Fagron	Ácido L-málico	15J09-B03-313987	40	20151106
Fagron	Ácido L-málico	15J09-B03-313987	40	20151106
Fagron	Ácido L-málico	16J06-B98-327269	40	20161117
Fagron	Ácido L-málico	16J06-B98-327269	40	20161117
Fagron	Ácido L-málico	17E23-B03-335458	40	20170621
Caelo	Agarikon (Laricifomes officinalis)	11024502	40	20110125
Caelo	Agarikon (Laricifomes officinalis)	13130602	48	1405003
Caelo	Agarikon (Laricifomes officinalis)	14190702	60	20140730
Caelo	Agarikon (Laricifomes officinalis)	14190706	60	20140730
Klenk	Agarikon (Laricifomes officinalis)	1061A120312	40	pending

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Agrimônia (Agrimonia eupatoria)	10325505	45	20101221
Caelo	Agrimônia (Agrimonia eupatoria)	11374004	40	20120125
Caelo	Alcachofra (Cynara scolymus), folha	12173302	40	20120706
Caelo	Alcachofra (Cynara scolymus), folha	13310707	40	20130930
Caelo	Alcaçuz	13068904	40	20130315
Caelo	Alcaçuz	14050601	60	from supplier
Caelo	Alcaçuz	13180904	60	pending
Bombastus	Alcarávia	23004707	30	20231023
Caelo	Alcarávia	13397104	40	AR-15-FG-001526-01
Caelo	Alcarávia	13397104	60	AR-15-FG-001527-01
Caelo	Alcarávia	13306006	60	AR-16-FG-000540-03
Caelo	Alcarávia	15097115	60	AR-17-FG-006649-01
Caelo	Alcarávia	22003284004	30	20230228
Euro OTC	Alginato de sódio	2305007	40	20230720*
Euro OTC	Alginato de sódio	2305007	20	20230720*
Fagron	Alginato de sódio	14G22-B99-297091	60	20140813
Gatt-Koller	Alginato de sódio	22J01179	40	20220714
Gatt-Koller	Alginato de sódio	22J01179	20	20220714
Caelo	Aloés, cabo	14087106	60	20140404
Caelo	Alumínio, óxido hidratadi	12163019	40	20120621
Caelo	Alumínio, óxido hidratadi	13119121	40	20130503
Caelo	Amêndoas amargas, inteiras	13220401	40	1406296
abcr GmbH	Amigdalina	1310927	40	from supplier
abcr GmbH	Amigdalina	1310579	40	from supplier
Auropure L...	Amigdalina, extrato de amêndoa amarga 98%	PA02099-160822	30	from supplier
Klenk	Amor-de-hortelão, cortada	4731B110809	40	20110930
Caelo	Anis	11370301	40	20120117
Klenk	Anis	2700A140129	60	20140926
Klenk	Anis	2700A160511	60	1708049
Caelo	Anis estrelado	11314104	10	20111121
Caelo	Anis estrelado, cortado	12226301	60	pending
Caelo	Anis estrelado, cortado	13041401	40	1403709
Caelo	Anis estrelado, cortado	15329302	60	AR-16-FG-004770-01
Caelo	Anis, esmagado	12111301	40	20120420
Caelo	Anis, pulverizado	11306203	40	20111110
Klenk	Arruda caprária, cortada	3901C110905	40	20111005
Caelo	Artemísia-vulgar	12016705	40	20120131
Fagron	Aspartame	21I21-B07-213840	40	20211216
Fagron	Aspartame	21I21-B07-213840	20	20211216
Fagron	Aspartato de magnésio dihidratado	15I24-B89-313231	60	AR-16-FG-008660-03
Fagron	Aspartato de magnésio dihidratado	15I24-B89-313231	60	20151016
Fagron	Aspartato de magnésio dihidratado	17C21-B05-333111	40	20170412
Fagron	Aspartato de magnésio dihidratado	18D23-B01-350069	40	20180625
Caelo	Aveia, palha	11280008	40	20111020
Fagron	Azitromicina	20F22-F01-372739	50	20200813
Fagron	Azitromicina	24C14-B02-231046	40	20240507
Fagron	Azitromicina	24C14-B02-231046	20	20240507
Roth	Azul brilhante R 250 (CI42660)	314217301	60	from supplier
Caelo	Babosa da montanha, pulverizada	11132115	40	1404400

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Babosa da montanha, pulverizada	11132115	40	20110520
Caelo	Bagas de zimbro	12028609	40	20120207
Caelo	Bagas de zimbro	13267210	40	20130828
Caelo	Bagas de zimbro, esmagado	12278903	40	1405296
Klenk	Bagas de zimbro, pulverizado	2894B130320	40	1411362
Klenk	Bagas de zimbro, pulverizado	2894B150922	60	1704439
Fagron	Benfotiamina	NL/BA/0152324	40	20240801*
Fagron	Benfotiamina	NL/BA/0152324	20	20240801*
Caelo	Bentonita	12237603	40	20120810
Fagron	Benzoato de metronidazol	22A17-B10-216356	40	20220607
Fagron	Benzoato de metronidazol	22A17-B10-216356	20	20220607
Gatt-Koller	Benzoato de sódio e cafeína	22J00803	40	20220530
Gatt-Koller	Benzoato de sódio e cafeína	23J01215	40	20230803
Gatt-Koller	Benzoato de sódio e cafeína	22J00803	20	20220530
Gatt-Koller	Benzoato de sódio e cafeína	23J01215	20	20230803
Fagron	Betaína cloridrato	BH20240119	40	20270117*
Fagron	Betaína cloridrato	BH20240119	20	20270117*
Caelo	Betônia (Stachys officinalis), cortada	12007205	40	20120118
Caelo	Betônia (Stachys officinalis), cortada	12007205	60	20120118
Caelo	Bicarbonato de sódio	23002402	40	20230919*
Caelo	Bicarbonato de sódio	23002402	20	20230919*
Euro OTC	Bicarbonato de sódio	1807021-01	40	20180725
Euro OTC	Bicarbonato de sódio	2202008	40	20220317*
Euro OTC	Bicarbonato de sódio	2302009	40	20230309*
Euro OTC	Bicarbonato de sódio	2306010	40	20230718*
Euro OTC	Bicarbonato de sódio	2202008	20	20220317*
Euro OTC	Bicarbonato de sódio	2302009	20	20230309*
Caelo	Bismuto, subnitrato (pesado)	181942	40	20181010*
Caelo	Black cohosh (Cimicifuga racemosa)	10281112	40	20101118
Caelo	Black cohosh (Cimicifuga racemosa)	13237901	40	pending
Caelo	Black cohosh (Cimicifuga racemosa)	13237903	40	20130812
Caelo	Botão de algodão americano	12027505	40	20120131
Klenk	Botão de algodão americano, esmagado	3266B130826	40	1410178
Klenk	Botão de algodão americano, esmagado	3266B150624	60	20150701
Fagron	Bromelaína	14F20-B03295501	40	pending
Fagron	Bromelaína	14F20-B03295501	60	20140701
Sigma-Aldrich	Bromelaína	BCBM1589V	40	from supplier
Sigma-Aldrich	Brometo de amônio	0000097635	40	not required
Caelo	Brometo de potássio	11208211	40	20110803
Caelo	Brometo de sódio	171191	40	20170510*
Caelo	Broto de pinheiro, cortado	11164708	60	20110610
Caelo	Broto de pinheiro, cortado	13256105	40	20130828
Fagron	Butirato de hidrocortisona	13I26-N01	60	AR-15-FG-000944-01
Fagron	Butirato de hidrocortisona	14D23-B01-296716	60	20140509
Fagron	Butirato de hidrocortisona	13I26-N01	60	20130920
Fagron	Butirato de hidrocortisona	16F20-B05-323903	40	20160805
Fagron	Butirato de hidrocortisona	15J12-B03-322394	40	20151028
Fagron	Butirato de hidrocortisona	16J21-B01-333229	40	20161206
Fagron	Butirato de hidrocortisona	16J21-B01-333229	40	20161206

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Butirato de hidrocortisona	14D23-B01-296716	48	20140509
Fagron	Butirato de hidrocortisona	13I26-N01	45	20130920
Fagron	Butirato de hidrocortisona	16F20-B05-323903	20	20160805
Fagron	Butirato de hidrocortisona	15J12-B03-322394	25	20151028
Fagron	Butirato de hidrocortisona	15J12-B03-322394	22	20151028
Fagron	Butirato de hidrocortisona	16J21-B01-333229	37	20161206
Fagron	Butirato de hidrocortisona	16J21-B01-333229	36	20161206
Caelo	Canela	12309902	40	pending
Caelo	Canela	13304414	40	20130912
Caelo	Canela	14175010	60	1505349
Caelo	Canela	16114401	60	1704441
Caelo	Carbacol	11150302	31	1401147
Fagron	Carbidopa monohidratada	23A26-B05-226465	40	20230330
Fagron	Carbidopa monohidratada	23I12-B04-236349	40	20231108
Fagron	Carbidopa monohidratada	23A26-B05-226465	20	20230330
Fagron	Carbidopa monohidratada	23I12-B04-236349	20	20231108
Euro OTC	Carbonato de magnésio, leve, básico	1711011-01	40	20171116
Euro OTC	Carbonato de magnésio, leve, básico	2201023	40	20220317*
Euro OTC	Carbonato de magnésio, leve, básico	2201023	20	20220317*
Caelo	Carbonato de potássio	180995	40	20180412*
Caelo	Carbonato de sódio deca-hidratado	173613	40	20180115*
Gatt-Koller	Carbonato de sódio deca-hidratado	23J00898	37	20230516
Gatt-Koller	Carbonato de sódio deca-hidratado	23J00898	28	20230516
Caelo	Carbonato de sódio monoidratado	16310205	40	20161221
Klenk	Cardamomo (Elettaria cardamomum), decorticado, pulverizado (especiaria)	2765A130524	60	AR-15-FG-015285-01
Caelo	Cardo-mariano, planta	10365601	40	20110111
Lycored corp.	Caromix	CMX-LLCV-011401	40	20140131
Caelo	Carvão ativado	181885	40	20180813*
Fagron	Carvedilol	22B21-F02-383500	40	20221111
Fagron	Carvedilol	22B21-F02-383500	20	20221111
Caelo	Casca de canela	13241807	40	20130905
Caelo	Casca de carvalho pulverizada	11235004	40	20110909
Caelo	Casca de cinchona, cortada	11238512	40	1403463
Caelo	Casca de cinchona, cortada	13031007	40	20130207
Caelo	Casca de cinchona, cortada	14009304	40	AR-15-FG-007677-01
Caelo	Casca de cinchona, cortada	15301903	60	AR-17-FG-007831-01
Caelo	Casca de frângula	12185901	40	20120710
Klenk	Casca de freixo, cortada	0871B110127	60	20110128
Caelo	Casca de hamamélis, cortada	12361301	40	20121213
Caelo	Casca de hamamélis, cortada	12361303	40	20121213
Caelo	Casca de lapacho, cortada	12239305	40	20120831
Caelo	Casca de limão, cortada	12217402	40	20120823
Caelo	Casca de olmo, cortada	10347205	60	20101223
Caelo	Casca de raiz de bérberis, cortada	12112601	40	20120430
Caelo	Casca de salgueiro	12185204	40	20120730
Caelo	Cascas de nozes	11325603	40	20111124

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Castanha-da-índia (Aesculus hippocastanum), folha	11063503	40	20110315
Caelo	Castoreum pulverizado	13410403	40	20131231
Caelo	Castoreum pulverizado	13410403	40	20131231
Caelo	Caule de doce-amarga (Solanum dulcamara), cortada	10375602	40	20110113
Caelo	Caule de doce-amarga (Solanum dulcamara), cortada	13254305	40	20130806
Caelo	Caule de ginja, cortado	12042302	40	1503570
Euro OTC	Caulim, pesado	2303011	40	20230412*
Euro OTC	Caulim, pesado	2303011	20	20230412*
Caelo	Caulim, vermelho	12093503	40	from supplier
Caelo	Cavalinha (Equisetum arvense), haste	10375515	40	20110114
Euro OTC	Cefaclor monoidratado	2311015	40	20240110*
Euro OTC	Cefaclor monoidratado	2310002	40	20240110*
Euro OTC	Cefaclor monoidratado	2311015	20	20240110*
Euro OTC	Cefaclor monoidratado	2310002	20	20240110*
Klenk	Celidônia maior	3731K120904	40	20120920
Caelo	Centaurea (Centaurium erythraea)	11097602	40	20110428
Klenk	Cerefólio (Anthriscus cerefolium), esmagado	3721A100329	40	20111128
Inresa	Cetoprofeno	F1300183	60	AR-15-FG-009572-01
Inresa	Cetoprofeno	F1300182	60	20150617
Caelo	Chá de Java (Orthosiphon stamineus)	12225702	40	20120809
Caelo	Chá de Java (Orthosiphon stamineus)	13258805	40	20130826
Klenk	Chá de Java (Orthosiphon stamineus)	2221B110718	40	20120605
Klenk	Chá verde (Camellia sinensis)	5100A100611	40	20120126
Caelo	Chicória, planta (Cichorium intybus)	12034303	60	20120228
Caelo	Chicória, planta (Cichorium intybus)	12354302	100	20121211
Fagron	Cimetidina	2403109C03	40	20270320*
Fagron	Cimetidina	2403109C03	20	20270320*
Fagron	Cinarizina	11L22-N13	40	20120104
Fagron	Cinarizina	13H01-N07	40	1402306
Fagron	Cinarizina	14D09-B01-294702	60	AR-16-FG-008930-01
Caelo	Cloreto de amônio	12356101	40	20121206
Euro OTC	Cloreto de amônio	1209013-01	40	20120928
Caelo	Cloreto de cálcio dihidratado	182411	35	20181022*
Caelo	Cloreto de cálcio dihidratado	23001613	40	20230717*
VWR Intern...	Cloreto de cálcio hexahidratado	22K294102	40	not required
Sigma-Aldrich	Cloreto de estanho(II) dihidratado	K54805315247	40	not required
Caelo	Cloreto de ferro (III) hexahidratado	12354703	40	1401391
Caelo	Cloreto de ferro (III) hexahidratado	22000819	40	20220323*
Caelo	Cloreto de ferro (III) hexahidratado	24002426	40	20241021*

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Cloreto de ferro (III) hexa-hidratado	22000819	10	20220323*
Caelo	Cloreto de ferro (III) hexa-hidratado	24002426	20	20241021*
VWR Intern...	Cloreto de magnésio 4,5-hidratado	22E054108	40	not required
Caelo	Cloreto de metilrosanilínio	12276308	40	1509299
Fagron	Cloreto de metilrosanilínio	13H28-N03	60	20130625
Fagron	Cloreto de metilrosanilínio	13H28-N03	60	AR-15-FG-004742-01
Fagron	Cloridrato de (R,S)-epinefrina	12H08-N03	40	no certificate available
Fagron	Cloridrato de (R,S)-epinefrina	14A22-B05-291560	60	no certificate available
Fagron	Cloridrato de (R,S)-epinefrina	16H23-B98-325052	40	20160913
Fagron	Cloridrato de amiodarona	18J26-B01-368910	40	20200429
Fagron	Cloridrato de amiodarona	18J26-B01-368910	20	20200429
Euro OTC	Cloridrato de betaína	2201015	40	not required
Euro OTC	Cloridrato de betaína	2309009	40	20231027*
Euro OTC	Cloridrato de betaína	2201015	10	not required
Euro OTC	Cloridrato de betaína	2309009	20	20231027*
Fagron	Cloridrato de betaína	13H13-N02	40	1402684
Gatt-Koller	Cloridrato de betaína	23J02134	40	20231121
Gatt-Koller	Cloridrato de betaína	23J02134	20	20231121
EDQM	Cloridrato de bromexina	5.0	40	CRS
Caelo	Cloridrato de buprenorfina	16143001	40	0718E-07774
Caelo	Cloridrato de buprenorfina	16143001	40	1919M-07774
Caelo	Cloridrato de buprenorfina	12172908	60	0814I-07774
Caelo	Cloridrato de buprenorfina	16143001	40	2017A-07774
Caelo	Cloridrato de buprenorfina	16143001	40	0718E-07774
Caelo	Cloridrato de buprenorfina	16143001	40	1919M-07774
Euro OTC	Cloridrato de ciclopentolato	2311002	40	20240322*
Euro OTC	Cloridrato de ciclopentolato	2409009	40	20241106*
Euro OTC	Cloridrato de ciclopentolato	2311002	20	20240322*
Euro OTC	Cloridrato de ciclopentolato	2409009	20	20241106*
Fagron	Cloridrato de cinchocaína	12F25-N10	40	1401148
Fagron	Cloridrato de cinchocaína	13G24-N05	40	20130826
Fagron	Cloridrato de drofenina	13I09-N05	40	20130524
Fagron	Cloridrato de drofenina	15G01-B04-323028	40	20150709
Fagron	Cloridrato de drofenina	15G01-B04-330979	40	AR-17-FG-015434-02
Fagron	Cloridrato de drofenina	15G01-B04-330979	40	20150709
Fagron	Cloridrato de drofenina	18A18-B99-345993	40	20180308
Euro OTC	Cloridrato de fexofenadina	2310018	20	20240222*
Flora Apot...	Cloridrato de levamisol	LV19305	40	from supplier
Fagron	Cloridrato de metformina	22C04-B02-219168	40	20220625
Fagron	Cloridrato de metformina	23H03-B10-234791	40	20230925
Fagron	Cloridrato de metformina	24B27-B04-239307	40	250201361
Fagron	Cloridrato de metformina	22C04-B02-219168	20	20220625
Fagron	Cloridrato de metformina	23H03-B10-234791	20	20230925
Fagron	Cloridrato de metformina	24B27-B04-239307	20	250201361
Caelo	Cloridrato de oxicodona	12268908	40	0914E-07734
Caelo	Cloridrato de oxicodona	12034515	40	0914F-07734
Caelo	Cloridrato de oxicodona	12268914	60	1416Q-07734
Caelo	Cloridrato de oxicodona	12268913	60	1416R-07734
Caelo	Cloridrato de oxicodona	15220205	40	2017A-07734
Caelo	Cloridrato de oxicodona	17270202	40	1919Q-07734
Caelo	Cloridrato de oxicodona	12268908	60	0914E-07734
Caelo	Cloridrato de oxicodona	12034515	60	0914F-07734
Caelo	Cloridrato de oxicodona	12268914	60	1416Q-07734
Caelo	Cloridrato de oxicodona	12268913	60	1416R-07734

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Cloridrato de oxicodona	15220205	40	2017A-07734
Caelo	Cloridrato de oxicodona	17270202	40	1919Q-07734
Caelo	Cloridrato de prometazina	13119214	60	20130506
Caelo	Cloridrato de prometazina	161466	40	20160621*
Caelo	Cloridrato de prometazina	17058601	40	20170310
Caelo	Cloridrato de prometazina	170586	40	20170310*
Fagron	Codeína monoidratada	12C05-N05	40	0814I-01280
Fagron	Codeína monoidratada	12C05-N05	60	0814I-01280
Caelo	Coentro	12080904	40	pending
Caelo	Coentro	13299403	40	1412548
Caelo	Coentro	16010212	60	AR-17-FG-015965-01
Caelo	Colofônia	15186804	60	AR-16-FG-005931-01
Caelo	Colofônia	161332	40	20160510*
Caelo	Colofônia	173014	40	20180102*
Caelo	Colofônia	192081	40	20190731*
Caelo	Cominho	11378308	30	20120124
Euro OTC	Concentrado seco de colecalciferol	1210051-01	40	1403341
Euro OTC	Concentrado seco de colecalciferol	1304016-02	40	20130425
Euro OTC	Concentrado seco de colecalciferol	1502021-01	60	20150309
Euro OTC	Concentrado seco de colecalciferol	1602019	40	20160307*
Euro OTC	Concentrado seco de colecalciferol	1701053	40	20170208*
Euro OTC	Concentrado seco de colecalciferol	1707027	40	20171020*
Euro OTC	Concentrado seco de colecalciferol	1802014	40	20180223*
Euro OTC	Concentrado seco de colecalciferol	1801038	40	20180206*
Euro OTC	Concentrado seco de colecalciferol	1806003	40	20180618*
Euro OTC	Concentrado seco de colecalciferol	1812010	40	20190114*
Euro OTC	Concentrado seco de colecalciferol	1901050	40	20190221*
Euro OTC	Concentrado seco de colecalciferol	1906009	40	20190619*
Caelo	Cravo	12095805	40	pending
Caelo	Cravo	16207804	60	1708676
Klenk	Cravo	1260A150916	40	1708050
Caelo	Cubeba (Piper cubeba)	11081903	40	20110404
Caelo	Cumaru (Dipteryx odorata)	12145101	40	20120604
Caelo	Cúrcuma, rizoma	11160403	60	20110628
Caelo	Cúrcuma, rizoma	12136503	40	1405295
Caelo	Cúrcuma, rizoma	13360202	40	1411363
Caelo	Dapsona	160735	60	20160405*
Caelo	Dapsona	16073502	40	20160405
Caelo	Dapsona	16073502	40	20160405
Caelo	Dapsona	170311	39	20170221*
Caelo	Dapsona	182792	40	20181214*
Caelo	Dapsona	191135	40	20190726*
Fagron	Deflazacorte	6017-240501	40	20240518*
Fagron	Deflazacorte	6017-240501	20	20240518*
Caelo	Dente-de-leão (Taraxacum officinale) , raiz	12363102	40	1403708
Caelo	Dente-de-leão (Taraxacum officinale) , raiz	13329701	40	20131017

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Dente-de-leão (Taraxacum officinale) , raiz	13329708	40	1411089
Klenk	Dente-de-leão (Taraxacum officinale) , raiz	6621B151029	60	AR-17-FG-007535-01
Caelo	Dente-de-Leão, planta sem raiz	11217109	40	20110824
Euro OTC	Dicloridrato de cetirizina	2210014	40	20230112*
Euro OTC	Dicloridrato de cetirizina	2210014	20	20230112*
Fagron	Dicloridrato de cetirizina	23C08-B01-227628	40	20230422
Fagron	Dicloridrato de cetirizina	23C08-B01-227628	20	20230422
Fagron	Dicloridrato de clorexidina	14A09-B03-290724	40	AR-15-FG-012308-01
Fagron	Dicloridrato de clorexidina	16C11-B02-324203	40	20160412
Fagron	Dicloridrato de clorexidina	16C11-B02-322510	40	20160412
Fagron	Dicloridrato de clorexidina	16C11-B02-329881	40	20160412
Caelo	Dicloridrato de quinina	16269603	40	1709386
Caelo	Dicloridrato de quinina	16269603	40	20161021
Caelo	Dicloridrato de quinina	162696	40	20161021*
Caelo	Dicloridrato de quinina	172129	40	20173008*
Caelo	Dicloridrato de quinina	172072	40	20170830*
Fagron	Difosfato de Cloroquina	24002C3RJ	40	20240124*
Fagron	Difosfato de Cloroquina	24002C3RJ	20	20240124*
Merck KGaA	Difosfato de sódio deca-hidratado	K55034491332	40	not required
Fagron	Dimenidrinato	21J13-B12-223576	40	20220117*
Fagron	Dimenidrinato	21J13-B12-223576	20	20220117*
Euro OTC	Dióxido de titânio	1708015-01	40	20170822
Euro OTC	Dissulfeto de selênio	1411011-02	40	20141211
Caelo	Echinacea pallida	12244501	40	20120817
Caelo	Echinacea pallida	14120602	40	20140417
EDQM	Econazol	1.0	10	CRS
Caelo	Endro, cortado	11295107	40	pending
Caelo	Endro, cortado	13007602	40	1402204
Caelo	Endro, cortado	13007610	40	20130208
Yino Pharma	Enoxaparina sódica	YN010232210003	40	20230524*
Yino Pharma	Enoxaparina sódica	YN010232210003	20	20230524*
Caelo	Epilobium angustifolium, planta	11347311	40	20111216
Caelo	Epilobium parviflorum	10326106	40	20101216
Caelo	Epilobium parviflorum	13355904	60	20140113
Klenk	Epilobium parviflorum	4721A140203	60	20140219
Caelo	Erva Alchemilla alpina, cortada	12147201	40	20120608
Caelo	Erva bolsa-de-pastor	11328208	40	20111205
Caelo	Erva cardo-santo, cortada	12038203	40	20120306
Caelo	Erva de borragem, cortada	11206712	40	20110822
Caelo	Erva de Ransom	12380801	40	1404538
Caelo	Erva de Ransom	13072801	40	20130326
Klenk	Erva Gelopsis, cortada	3911A090219	40	20120426
Klenk	Erva grega das montanhas, cortada	4511K130314	40	20130402
Klenk	Erva-doce	2870A110412	40	pending
Klenk	Erva-doce	2870A130304	40	1405154
Bombastus	Erva-doce, amarga	289870	60	AR-15-FG-008161-01
Bombastus	Erva-doce, amarga	24000576	30	20240129
Caelo	Erva-doce, amarga	12094708	40	pending
Caelo	Erva-doce, amarga	12167102	40	20120705
Caelo	Erva-doce, amarga	13413702	40	1412549
Caelo	Erva-doce, amarga	14376403	60	20150108
Caelo	Erva-doce, amarga	161603	60	20160718*
Caelo	Erva-doce, amarga	17020610	40	1708048

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Erva-doce, amarga	23002233002	30	20231212
Klenk	Erva-doce, amarga	2880N120418	40	1412547
Klenk	Erva-doce, amarga	2880N120418	40	AR-15-FG-002805-02
Klenk	Erva-doce, amarga	2860A140613	60	AR-15-FG-008160-01
EDQM	Estearato de eritromicina	1.2	40	CRS
Bombastus	Estigma de milho	274920	40	66662
Caelo	Estigma de milho	10325906	40	20101217
Caelo	Estigma de milho	13381501	40	20140103
Klenk	Estigma de milho	5581A111206	40	20111214
EDQM	Estolato de eritromicina	1.4	40	CRS
Fagron	Estolato de Eritromicina	EV/EE-085/24	40	20240803*
Fagron	Estolato de Eritromicina	EV/EE-085/24	20	20240803*
Caelo	Estróbilo de lúpulo	12008305	40	20120213
Caelo	Estróbilo de lúpulo	12221802	40	20120817
Caelo	Estróbilo de lúpulo	23001009005	30	20230823
Klenk	Eufrásia	3871B100713	40	20100721
Euro OTC	Extrato de cúrcuma 95%	L1408013	60	20140815
Dr. Behr	Extrato de inhame	WE14020005-05	40	pending
Euro OTC	Extrato de olíbano 80%	1308020-01	60	8958
Euro OTC	Extrato de olíbano 80%	1602008	60	20160215*
Euro OTC	Extrato de olíbano 80%	1602008	60	20160215*
Euro OTC	Extrato de olíbano 80%	1611023-01	60	9889
Caelo	Extrato de própolis (96%) 2:1	11124120	40	1403460
Caelo	Extrato de própolis (96%) 2:1	13396103	40	20131212
Caelo	Extrato de própolis (96%) 2:1	13396103	40	20131212
Euro OTC	Extrato de semente de Griffonia	1810009	40	20181025*
Fagron	Extrato de semente de Griffonia (L-5 Hidroxitriptofano)	20240412	40	not required
Fagron	Extrato de semente de Griffonia (L-5 Hidroxitriptofano)	2024020	40	not required
Fagron	Extrato de semente de Griffonia (L-5 Hidroxitriptofano)	20240414	40	not required
Fagron	Extrato de semente de Griffonia (L-5 Hidroxitriptofano)	20240412	20	not required
Fagron	Extrato de semente de Griffonia (L-5 Hidroxitriptofano)	2024020	40	not required
Fagron	Extrato de semente de Griffonia (L-5 Hidroxitriptofano)	20240414	20	not required
Euro OTC	Extrato seco de garra-do-diabo	2101020	40	20210203*
Euro OTC	Extrato seco de garra-do-diabo	1210003-02	40	1707472
Euro OTC	Extrato seco de garra-do-diabo	1210003-02	40	20151102
Euro OTC	Extrato seco de garra-do-diabo	1210003-02	40	20151102
Caelo	Extrato seco de Ginkgo, refinado, quantificado	12192505	40	1403672
Caelo	Feno-grego	11313204	40	20111122
Caelo	Feno-grego pulverizado	12149605	40	20120629

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Feno-grego pulverizado	15308704	60	AR-17-FG-006625-01
Klenk	Feno-grego pulverizado	7264B130205	40	1408080
Klenk	Feno-grego pulverizado	7264A151001	60	AR-16-FG-014493-01
Caelo	Fenol	23002846	40	20231108*
Caelo	Fenol	24001307	40	20240701*
Caelo	Fenol	24001307	20	20240701*
Fagron	Fenolftaleína	20G24-F01-375331	40	20201202
Fagron	Fenolftaleína	22J07-B02-227243	40	20221102
Fagron	Fenolftaleína	20G24-F01-375331	20	20201202
Fagron	Fenolftaleína	22J07-B02-227243	20	20221102
Klenk	Filipenda ulmaria	4541A120313	60	20120327
Caelo	Flor de abrunheiro	12178101	40	20120718
Caelo	Flor de arnica	11285702	40	20111118
Caelo	Flor de arnica	11259801	40	20110923
Bombastus	Flor de calêndula	24002342	30	20240528
Caelo	Flor de calêndula	11221404	40	20110930
Caelo	Flor de calêndula	22003249004	30	20221214
Caelo	Flor de camomila para banho	12115805	40	from supplier
Bombastus	Flor de camomila-vulgar	24004030	30	20240926
Caelo	Flor de camomila-vulgar	12294804	40	20121113
Caelo	Flor de camomila-vulgar	24100110001	30	20241031
bubatzbros.de	Flor de cannabis	BBCD11-092023	30	00080
bubatzbros.de	Flor de cannabis	BBMK11-092023	30	00081
Cansativa	Flor de cannabis	06051825121-2-P2	30	00001
Cansativa	Flor de cannabis	ICC230402	30	00002
Cansativa	Flor de cannabis	ICC230503	30	00003
Cansativa	Flor de cannabis	WES230301	30	00004
Cansativa	Flor de cannabis	GG4230303Y	30	00005
Cansativa	Flor de cannabis	ZRP230101	30	00006
Cansativa	Flor de cannabis	28202	30	00007
Cansativa	Flor de cannabis	13302	30	00008
Cansativa	Flor de cannabis	06051822121-3-P1	30	00009
Cansativa	Flor de cannabis	02209916122-1-P3	30	00010
Cansativa	Flor de cannabis	C038	30	00011
Cansativa	Flor de cannabis	C086	30	00012
Cansativa	Flor de cannabis	C082	30	00013
Cansativa	Flor de cannabis	BKS2290001-1R1-6	30	00014
Cansativa	Flor de cannabis	22K07FP23A18	30	00015
Cansativa	Flor de cannabis	22K28FB23C15	30	00016
Cansativa	Flor de cannabis	22I05EY22K30	30	00017
Cansativa	Flor de cannabis	22H08FR22I28	30	00018
Cansativa	Flor de cannabis	AKH2311001-1R1-6	30	00019
Cansativa	Flor de cannabis	S87B2056CA-2R3-6	30	00020
Cansativa	Flor de cannabis	91K2137CA-1R2-6	30	00021
Cansativa	Flor de cannabis	LSK2216001-1R2-6	30	00022
Cansativa	Flor de cannabis	22TC06HB010102	30	00023
Cansativa	Flor de cannabis	22GS02SI010202	30	00024
Cansativa	Flor de cannabis	C091	30	00025
Cansativa	Flor de cannabis	D016	30	00026
Cansativa	Flor de cannabis	D013	30	00027
Cansativa	Flor de cannabis	D032	30	00028
Cansativa	Flor de cannabis	030122LS-T22/10	30	00029
Cansativa	Flor de cannabis	P22057FT	30	00030
Cansativa	Flor de cannabis	P22055FT	30	00031
Cansativa	Flor de cannabis	P22050FT-A	30	00032
Cansativa	Flor de cannabis	02209951121-2-P1	30	00033
Cansativa	Flor de cannabis	02209910122-3-P1	30	00034
Cansativa	Flor de cannabis	CMNG23FSRE032877	30	00035
Cansativa	Flor de cannabis	02209912122-1-P3	30	00036

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Cansativa	Flor de cannabis	22GS12WLC010105	30	00037
Cansativa	Flor de cannabis	22GS12MG010102	30	00038
Cansativa	Flor de cannabis	22GS15BB010202	30	00039
Cansativa	Flor de cannabis	22GS02MK020102	30	00040
Cansativa	Flor de cannabis	2203GG010402	30	00041
Cansativa	Flor de cannabis	21GS11HB040104	30	00042
Cansativa	Flor de cannabis	2203PD010105	30	00043
Cansativa	Flor de cannabis	22TC08HB010103	30	00044
Cansativa	Flor de cannabis	21GS06ISS040102	30	00045
Cansativa	Flor de cannabis	21GS06ISS040102	30	00046
Cansativa	Flor de cannabis	21GS06MG030106	30	00047
Cansativa	Flor de cannabis	22GS10PPS010102	30	00048
Cansativa	Flor de cannabis	22TC05SI010102	30	00049
Cansativa	Flor de cannabis	2GS02BB010105	30	00050
Cansativa	Flor de cannabis	22GS02GWO010103	30	00051
Cansativa	Flor de cannabis	22TC07PK010103	30	00052
Cansativa	Flor de cannabis	C060	30	00053
Cansativa	Flor de cannabis	02209920122-1-P1	30	00054
Cansativa	Flor de cannabis	02209913122-1-P1	30	00055
Cansativa	Flor de cannabis	P22058FT	30	00056
Cansativa	Flor de cannabis	22GS12WLC010105	30	00057
Cansativa	Flor de cannabis	TRP230603	30	00058
Cansativa	Flor de cannabis	GG4230506	30	00059
Cansativa	Flor de cannabis	28302	30	00060
Cansativa	Flor de cannabis	28303	30	00061
Cansativa	Flor de cannabis	2306605	30	00062
Cansativa	Flor de cannabis	D043	30	00063
Cansativa	Flor de cannabis	VA0163-2301	30	00064
Cansativa	Flor de cannabis	06051821121-1-P1	30	00065
Cansativa	Flor de cannabis	ICC230503	30	00089
Cansativa	Flor de cannabis	WES230301	30	00090
Cansativa	Flor de cannabis	ZRP230101	30	00091
Cansativa	Flor de cannabis	28202	30	00092
Cansativa	Flor de cannabis	C038	29	00093
Cansativa	Flor de cannabis	S87B2056CA-2R3-6	30	00097
Cansativa	Flor de cannabis	LSK2216001-1R2-6	30	00098
Cansativa	Flor de cannabis	D013	30	00099
Cansativa	Flor de cannabis	D032	31	00100
Cansativa	Flor de cannabis	P22057FT	30	00101
Cansativa	Flor de cannabis	P22050FT-A	30	00102
Cansativa	Flor de cannabis	22GS12WLC010105	30	00103
Cansativa	Flor de cannabis	02209913122-1-P1	30	00104
Cansativa	Flor de cannabis	P22058FT	30	00105
Cansativa	Flor de cannabis	22GS12WLC010105	30	00106
Cansativa	Flor de cannabis	TRP230603	30	00107
Cansativa	Flor de cannabis	28302	30	00108
Cansativa	Flor de cannabis	28303	30	00109
Cansativa	Flor de cannabis	2306605	20	00110
Cansativa	Flor de cannabis	D043	30	00111
Cansativa	Flor de cannabis	C038	31	00112
Cansativa	Flor de cannabis	HSK2145CA-3R2-6	30	00116
Cansativa	Flor de cannabis	LSK2216001-1R2-6	30	00117
Cansativa	Flor de cannabis	D032	30	00118
Cansativa	Flor de cannabis	P22057FT	30	00119
Cansativa	Flor de cannabis	P22050FT-A	30	00120
Cansativa	Flor de cannabis	22GS12WLC010105	30	00121
Cansativa	Flor de cannabis	P22058FT	30	00122
Cansativa	Flor de cannabis	28302	30	00123
Cansativa	Flor de cannabis	2306605	30	00124
Cansativa	Flor de cannabis	D043	30	00125

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Cansativa	Flor de cannabis	06051825121-2-P2	30	00126
Cansativa	Flor de cannabis	06051822121-3-P1	30	00127
Cansativa	Flor de cannabis	22GS12MG010102	30	00128
Cansativa	Flor de cannabis	22GS15BB010202	30	00129
Cansativa	Flor de cannabis	D013	30	00130
Cansativa	Flor de cannabis	22GS12WLC010105	40	00131
CBD NOL	Flor de cannabis	CNRK8-092023	30	00132
CBD NOL	Flor de cannabis	CNSLH5-092023	30	00133
CBD NOL	Flor de cannabis	CNC5-092023	30	00134
CBD NOL	Flor de cannabis	CNPK6-092023	30	00135
CBD NOL	Flor de cannabis	CNAH6-092023	30	00136
CBD NOL	Flor de cannabis	CNPE6-092023	30	00137
CBD NOL	Flor de cannabis	CNBB0-092023	30	00138
CBD NOL	Flor de cannabis	CNBA10-092023	30	00139
Hanfgarten.at	Flor de cannabis	HCB000020	30	00082
Hanfgarten.at	Flor de cannabis	HCB000019	37	00083
Hanfgarten.at	Flor de cannabis	HCB000021	30	00084
Hanfgarten.at	Flor de cannabis	HCB000014	31	00085
Hanfgarten.at	Flor de cannabis	HCB000040	31	00086
Hanfgarten.at	Flor de cannabis	HCB000015	40	00087
Hanfgarten.at	Flor de cannabis	HCB000046	30	00088
happy420.de	Flor de cannabis	100000318	30	00066
happy420.de	Flor de cannabis	100000019	30	00067
happy420.de	Flor de cannabis	100000814	30	00068
happy420.de	Flor de cannabis	100000017	30	00069
happy420.de	Flor de cannabis	100000024	30	00070
happy420.de	Flor de cannabis	100000365	30	00071
happy420.de	Flor de cannabis	100000167	30	00072
justbob	Flor de cannabis	ES239230223	30	00073
justbob	Flor de cannabis	ES259061222	30	00074
justbob	Flor de cannabis	ES326090523	30	00075
Luckyhemp.de	Flor de cannabis	BN-0033-03	30	00076
Luckyhemp.de	Flor de cannabis	BN-0009-03	30	00077
Luckyhemp.de	Flor de cannabis	BN-0003-03	30	00078
Luckyhemp.de	Flor de cannabis	BN-0041-03	30	00079
Caelo	Flor de centáurea	10291105	40	pending
Caelo	Flor de centáurea	13241902	60	AR-15-FG-005838-01
Caelo	Flor de espinheiro-branco	10157201	40	20100701
Caelo	Flor de espinheiro-branco	13010403	40	20130130
Caelo	Flor de hibisco	12007311	60	20120124
Caelo	Flor de hibisco	11036509	60	20110303
Caelo	Flor de hibisco, cortada	10244508	60	20100917
Caelo	Flor de jasmim	12143201	40	20120606
Bombastus	Flor de lavanda	24000229	30	20240111
Caelo	Flor de lavanda	12088003	60	20120411
Caelo	Flor de lavanda	13336005	40	from supplier
Caelo	Flor de lavanda	23001761001	30	20231129
Caelo	Flor de malva	12187405	40	20120719
Caelo	Flor de prímula	11206806	100	20110809
Caelo	Flor de prímula	11268002	40	20111007
Caelo	Flor de rosa vermelha	11299204	40	from supplier
Caelo	Flor de tília	11086305	55	20110420
Caelo	Flor de ulmária, separada	12275701	40	20121023
Caelo	Flor de urtiga-branca	11371604	40	20120103
Caelo	Flor de urze, separada	10270508	40	20101018
Caelo	Flor de verbasco	11366403	40	20120105
Caelo	Flor de verbasco, cortada	11233402	60	20110914
Caelo	Flor de vulnerária, grosseiramente separada	10249206	40	20100928
Audor	Fluconazol	AP061502911F	60	AR-16-FG-008733-01

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Audor	Fluconazol	AP061502911F	40	AR-16-FG-014225-01
Audor	Fluconazol	AP061502911F	40	20150821
Audor	Fluconazol	APAFLNC0217023F	40	20170421
Audor	Fluconazol	AP061502911F	60	20150821
Audor	Fluconazol	AP061502911F	40	20150821
Audor	Fluconazol	AP061502911F	40	20150821
Bombastus	Folha de alecrim	23004436	30	20231017
Caelo	Folha de alecrim	14159601	60	20140617
Caelo	Folha de alecrim	23001738001	30	20231124
Klenk	Folha de alecrim	2261A131118	60	AR-15-FG-008499-01
Caelo	Folha de amora	11030707	40	20110303
Galke	Folha de amora	18060	40	20111021
Caelo	Folha de arando vermelho, cortada	11334302	40	20111129
Caelo	Folha de bétula	12193105	40	20120710
Caelo	Folha de boldo	13367904	40	20131122
Galke	Folha de boldo	19855	40	20120727
Klenk	Folha de boldo	1911A100714	40	20111214
Caelo	Folha de buchu	12034903	40	20120221
Caelo	Folha de cardo aquático, cortada	12226101	40	20120809
Caelo	Folha de Damiana, cortada	11026608	40	20110221
Bombastus	Folha de erva-cidreira	24001976	30	20240423
Caelo	Folha de erva-cidreira	12032318	40	20120302
Caelo	Folha de erva-cidreira	24100001001	30	20240502
Galke	Folha de erva-cidreira	22218	40	from supplier
Klenk	Folha de erva-cidreira	2161A090630	130	20120328
Klenk	Folha de erva-cidreira	2161A121029	55	20121113
Caelo	Folha de espinheiro-branco com flores	10273515	40	20101028
Caelo	Folha de espinheiro-branco com flores	10273513	40	20101028
Caelo	Folha de espinheiro-branco com flores	13276706	40	20130927
Galke	Folha de espinheiro-branco com flores	21126	40	20121109
Caelo	Folha de framboesa	12362701	40	20121219
Caelo	Folha de freixo, cortada	11031303	40	20110224
Caelo	Folha de ginkgo	12151703	40	20120613
Caelo	Folha de ginkgo	13340904	40	1411088
Caelo	Folha de ginkgo	13340907	60	20131028
Caelo	Folha de ginkgo	16281501	60	1708047
Caelo	Folha de ginkgo	24100105001	30	20241011
Klenk	Folha de ginkgo	2461B220718-01	30	20220802
Caelo	Folha de groselha, cortada	12168804	40	20120711
Caelo	Folha de hamamélis	10102915	40	20100517
Caelo	Folha de hamamélis	13269902	40	1405176
Caelo	Folha de hamamélis	13269904	40	20130924
Caelo	Folha de hera, cortada	11229505	40	20110829
Caelo	Folha de hera, cortada	13276304	40	20130913
Bombastus	Folha de hortelã-pimenta	24003080	30	20240716
Caelo	Folha de hortelã-pimenta	11294401	40	20111104
Caelo	Folha de hortelã-pimenta	12321503	130	20121026
Caelo	Folha de hortelã-pimenta	13288303	40	20131002
Caelo	Folha de hortelã-pimenta	24100035002	30	20240717
Galke	Folha de hortelã-pimenta	20244	40	20120518
Galke	Folha de hortelã-pimenta	19537	40	from supplier
Caelo	Folha de louro	12299103	40	20121108
Klenk	Folha de louro, pulverizada	2124A110329	40	1411032
Klenk	Folha de louro, pulverizada	2124A110329	60	20140310

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Folha de malva	12153403	40	20120614
Caelo	Folha de marshmallow	12328206	40	20121114
Caelo	Folha de mate	11091707	40	20110428
Caelo	Folha de mate	13118004	40	20130506
Caelo	Folha de mate	24100015001	30	20240610
Galke	Folha de mate	21684	40	from supplier
Caelo	Folha de mirtilo	12140206	40	20120605
Caelo	Folha de morango	11117903	40	20110428
Klenk	Folha de morango	2031B110224	40	20110304
Klenk	Folha de morango	2031B120925	40	20121005
Caelo	Folha de nogueira	11103007	40	1403091
Caelo	Folha de oliveira	11270106	40	20111013
Caelo	Folha de oliveira	12316808	60	AR-15-FG-001051-01
Klenk	Folha de sabugueiro, cortada	2321B130221	60	20130226
Caelo	Folha de sálvia	11347503	40	20120102
Bombastus	Folha de sene	24000491	30	20240130
Caelo	Folha de sene	12273106	40	20120927
Caelo	Folha de sene	23001268010	30	20230714
Caelo	Folha de sene pulverizada	11193307	120	pending
Caelo	Folha de sene pulverizada	12369908	40	1408079
Klenk	Folha de sene pulverizada	2334B130606	60	AR-15-FG-015212-01
Caelo	Folha de urtiga	12184702	40	20120628
Galke	Folha de urtiga	21238	40	from supplier
Caelo	Folha de uva-ursi	12186502	40	20120705
Caelo	Folha de verbena-limão, cortada	12137505	40	20120605
Caelo	Folha de verbena-limão, cortada	12137503	40	20120605
Caelo	Fosfato básico de potássio	12366501	40	10401307
Caelo	Fosfato básico de potássio	21001529	50	20210712*
Th. Geyer	Fosfato de colamina de cálcio	36986	40	from supplier
Th. Geyer	Fosfato de Mg-Ca-K-colamina	54610	40	from supplier
Th. Geyer	Fosfato de Mg-Ca-K-colamina	54610	40	from supplier
Caelo	Fosfato de sódio dibásico dodeca-hidratado	22000404	40	20220211*
Caelo	Fosfato de sódio dibásico dodeca-hidratado	22001508	40	20220531
Caelo	Fosfato de sódio dibásico dodeca-hidratado	22002975	40	20220930*
Caelo	Fosfato de sódio dibásico dodeca-hidratado	23002592	40	20231024*
Caelo	Fosfato de sódio dibásico dodeca-hidratado	24000747	40	20240507*
Caelo	Fosfato de sódio dibásico dodeca-hidratado	22000404	20	20220211*
Caelo	Fosfato de sódio dibásico dodeca-hidratado	22001508	20	20220531
Caelo	Fosfato de sódio dibásico dodeca-hidratado	22002975	20	20220930*
Caelo	Fosfato monobásico de magnésio tri-hidratado	12181911	40	20120716
Caelo	Fosfato monobásico de sódio hepta-hidratado	12109002	40	20120424
Caelo	Fosfato monobásico de sódio hepta-hidratado	21003087	40	20210927*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Fosfato monobásico de sódio hepta-hidratado	21003087	20	20210927*
Euro OTC	Fosfato tricálcico	1206002-01	40	1402298
Caelo	Fruto da alcarávia, esmagada	13367101	40	20130503
Caelo	Fruto da alcarávia, esmagada	14358801	60	AR-15-FG-014914-01
Caelo	Fruto da alcarávia, esmagada	16073201	60	AR-17-FG-006648-01
Caelo	Fruto da sene tinnevelly	12267605	40	20120921
Caelo	Fruto da sene tinnevelly	11154404	40	20110607
Caelo	Fruto da sene tinnevelly	13395106	40	20140106
Caelo	Fruto de bérberis	11058309	40	pending
Caelo	Fruto de bérberis	12217109	60	pending
Caelo	Fruto de bérberis	14057312	60	1508391
Caelo	Fruto do agnocasto	12274003	40	1501649
Caelo	Fruto do agnocasto	13193401	40	AR-15-FG-006453-01
Caelo	Fruto do agnocasto	15318705	60	pending
Klenk	Fruto do aipo	7140A130625	40	1405177
Klenk	Fruto do aipo	7140A230110-01	30	20230214
Caelo	Fruto do cardamomo	11309107	40	20111111
Caelo	Fruto do cardamomo	13260504	40	20130906
Caelo	Fruto do cardo-mariano	11126703	40	20110608
Caelo	Fruto do cardo-mariano	13342002	40	from supplier
Caelo	Fruto do endro (Anethum graveolens)	12289901	40	1403464
Caelo	Fruto do endro (Anethum graveolens)	12342906	40	20121206
Caelo	Fruto do endro (Anethum graveolens)	14018705	60	pending
Caelo	Fruto do endro (Anethum graveolens)	23001474001	30	20231010
Klenk	Fruto do endro (Anethum graveolens)	2680A170222	60	20170308
Caelo	Fruto do espinheiro-branco	11183010	40	20110701
Caelo	Fruto do espinheiro-branco	11278205	30	20111025
Caelo	Fruto do sabugueiro	12267807	40	1403466
Caelo	Fruto do sabugueiro	13367704	40	1410179
Klenk	Fruto do sabugueiro	3010A120202	40	pending
Euro OTC	Fumarato de cetotifeno	2109027	50	20211026*
Euro OTC	Fumarato de cetotifeno	2304008	40	20230420*
Euro OTC	Fumarato de cetotifeno	2109027	10	20211026*
Euro OTC	Fumarato de cetotifeno	2304008	20	20230420*
Caelo	Fumarato de dimetila	13269801	60	1506634
Euro OTC	Fumarato de dimetila	1410013-01	60	20141125
Euro OTC	Fumarato de dimetila	1601013-01	40	20160204
Fagron	Fumarato monobásico de etila	14C12-B07-292760	60	1410436
Fagron	Fumarato monobásico de etila	14C12-B07-292760	60	20140417
Euro OTC	Fumarato monobásico de etila cálcio	1310029-01	60	20131126
Euro OTC	Fumarato monobásico de etila cálcio	1306012-01	60	1505456
Euro OTC	Fumarato monobásico de etila cálcio	1510005	60	20151030*
Euro OTC	Fumarato monobásico de etila cálcio	1601011	60	20160114*
Euro OTC	Fumarato monobásico de etila cálcio	2001042	40	20200331*

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Fumarato monobásico de etila cálcio	13B25-N08	60	1411090
Euro OTC	Fumarato monobásico de etila magnésio	1306014-01	60	20130805
Euro OTC	Fumarato monobásico de etila magnésio	1510006	60	20151030*
Euro OTC	Fumarato monobásico de etila magnésio	1601010	60	20160114*
Euro OTC	Fumarato monobásico de etila magnésio	1510006-01	40	AR-18-FG-000547-01
Fagron	Fumarato monobásico de etila magnésio	13G10-N01	60	1411091
Caelo	Fumitória	12103402	40	20120425
Fagron	Fusidato de sódio	23A04-B10-219743	40	20230209
Fagron	Fusidato de sódio	23F12-B05-22913	40	20230705
Fagron	Fusidato de sódio	23A04-B10-219743	20	20230209
Fagron	Fusidato de sódio	23F12-B05-22913	20	20230705
Caelo	Galium odoratum	10375812	30	20110114
Caelo	Galium verum	11265103	40	20111006
Klenk	Galium verum	3921B101012	40	20111216
Caelo	Gengibre	14120701	40	20140516
Caelo	Gengibre	13321904	40	20131016
Klenk	Gengibre, descascado, pulverizado	6954B140724	60	AR-15-FG-014915-01
Klenk	Gengibre, descascado, pulverizado	6954B150325	60	1606616
Klenk	Gengibre, descascado, pulverizado	6954B170127	60	1708675
Fagron	Ginkgo biloba extrato seco (padronizado para conter no mínimo 24% de flavonoides totais)	24H27-B082	40	20240925*
Fagron	Ginkgo biloba extrato seco (padronizado para conter no mínimo 24% de flavonoides totais)	24H27-B082	20	20240925*
Caelo	Ginseng siberiano, cortado	10381814	30	20110113
Euro OTC	Gluconato de cobre (II)	2202011	40	20220301*
Euro OTC	Gluconato de cobre (II)	2202011	40	20220301*
Caelo	Groselha	14212502	60	20140829
Caelo	Groselha	14212509	60	20140829
Caelo	Guaiaco (madeira)	11352001	40	1406340
Caelo	Guaiaco (madeira)	11352012	40	20111222
Caelo	Guaiaco (madeira)	13343802	40	20131113
Fagron	Hemifumarato de bisopropol	24I18-B04-003143	40	20241003
Fagron	Hemifumarato de bisopropol	24I18-B04-003143	20	20241003
Fagron	Hemi-hidrato de clorobutanol	14A06-B31-290310	60	1412458
EDQM	Hemissuccinato de hidrocortisona	3.0	40	CRS
EDQM	Hemissuccinato de metilprednisolona	3.0	40	CRS
Caelo	Hena pulverizada	12122302	40	from supplier
Caelo	Hena pulverizada	12267304	40	from supplier
Caelo	Herniária	13007505	40	1403462
Caelo	Herniária	14005309	60	20140203
Caelo	Herniária	20003289005	30	20201130
Audor	Hialuronato de sódio	AP30101404H	60	20141203
Audor	Hialuronato de sódio	AP30101702H	40	1802037
Caelo	Hialuronato de sódio	172347	40	20171004*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Euro OTC	Hialuronato de sódio	L1302028-01	40	1403532
Euro OTC	Hialuronato de sódio	L1302028-01	60	20130314
Kraeber & ...	Hialuronato de sódio	3462	40	20180723
Kraeber & ...	Hialuronato de sódio	3829	40	2104160
Kraeber & ...	Hialuronato de sódio	3897	40	20200408
Sigma-Aldrich	Hidrato de hidróxido de alumínio	102465140	40	not required
Sigma-Aldrich	Hidrogênio fosfato dissódico	102544017	40	not required
Caelo	Hidróxido de magnésio	16253301	30	20160921
Caelo	Hidróxido de potássio	180083	40	20180118*
Fagron	Índigo-carmim	13K12-N01	40	1601099
Spinnrad	Inulina	1112300433	40	from supplier
Caelo	Iodeto de potássio	11090222	40	20110415
Caelo	Iodeto de sódio	161701	40	20160706*
Caelo	Iodo	181635	40	20180704*
EDQM	Isoconazol	1.1	40	CRS
Caelo	Isomalte	170812	40	20170421*
Sigma-Aldrich	Isonicotinato de dexametasona	Y0000538	40	CRS
Fagron	Ivermectina	22E06-H05-00747	40	20220511
Fagron	Ivermectina	22E06-H05-00747	20	20220511
FSA Chemicals	Ivermectina	23J18-AP24014	20	241107538
Euro OTC	Kaliumorotat	1203038V-02	40	from supplier
Flora Apot...	Kaliumorotat	ORK00119	40	from supplier
Fagron	L-5-hidroxitriptofano	21G12-B06-213943	40	20211103
Fagron	L-5-hidroxitriptofano	23G12-B14-231034	40	20230817
Fagron	L-5-hidroxitriptofano	21G12-B06-213943	11	20211103
Fagron	L-5-hidroxitriptofano	23G12-B14-231034	20	20230817
Caelo	Laranja-amarga (Citrus aurantium), flores (pétalas)	12266605	40	20120907
Caelo	Laranja-amarga (Citrus aurantium), flores (pétalas)	12266703	40	20120907
Caelo	Laranja-amarga, casca	12067405	40	20120327
Klenk	Leonurus cardiaca	4071A121211	40	20130104
Caelo	Levisticum officinale	11181609	40	20110629
Caelo	Linhaça	12092102	60	20120402
Caelo	Linhaça	13296703	40	20131008
Fagron	Losartana potássica	D5440-24-006	20	20240410*
Caelo	Maçã, cortada	11229807	60	from supplier
Fagron	Macrogol 6000, pó	14C11-B01-296014	60	20140324
Fagron	Macrogol 6000, pó	14J17-B01-309247	60	20141027
Fagron	Macrogol 6000, pó	14J17-B01-309247	60	AR-16-FG-011486-01
Caelo	Maná	11308907	60	20111117
Caelo	Maná	13127007	40	20130424
Caelo	Maná, pulverizado	11308807	40	1403534
Caelo	Maná, pulverizado	14001401	40	20140115
Caelo	Manjericão, triturado	12066404	50	20120321
Klenk	Maracujá, planta	4231A120329	40	20120419
Caelo	Margarida, flor	11068306	40	20110323
Caelo	Mentha spicata, folha	12133906	40	20120516
Fagron	Mesilato de diidroergotamina	22A11-F01-384535	40	20220328
Fagron	Mesilato de diidroergotamina	22A11-F01-384535	20	20220328
Gatt-Koller	Mesilato de diidroergotamina	22J02560	40	20230109
Gatt-Koller	Mesilato de diidroergotamina	22J02560	20	20230109
Fagron	Mesilato de Doxazosina	DM0060624	40	20240705*
Fagron	Mesilato de Doxazosina	DM0060624	20	20240705*

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Metabissulfito de potássio	12325906	40	20121106
Dr. K. Hol...	Miconazol	029C064	40	20190415
Fagron	Midazolam	13K05-N01	40	0914E-07393
Fagron	Midazolam	14C12-B31-313222	60	1516A-07393
Fagron	Midazolam	16J03-B09-326963	40	1917Q-07393
Fagron	Midazolam	17J16-B01-342518	40	1919I-07393
Fagron	Midazolam	13K05-N01	60	0914E-07393
Fagron	Midazolam	14C12-B31-313222	60	1516A-07393
Fagron	Midazolam	16J03-B09-326963	30	1917Q-07393
Fagron	Midazolam	17J16-B01-342518	40	1919I-07393
Caelo	Mil-folhas (Achillea millefolium)	12267703	40	20120921
Caelo	Mirra	12269901	40	1403470
Klenk	Mirra	3355B120628	40	AR-15-FG-000945-01
MEDICHEM S.A.	Mirtazapina	A-180132	50	20180312
MEDICHEM S.A.	Mirtazapina	A-210100	50	20210211
MEDICHEM S.A.	Mirtazapina	2024A152	40	20241023
MEDICHEM S.A.	Mirtazapina	A-180132	50	20180312
MEDICHEM S.A.	Mirtazapina	A-210100	50	20210211
MEDICHEM S.A.	Mirtazapina	2024A152	40	20241023
Caelo	Mistura de óxido de zinco-talco 1:1	181487	40	20180702*
Euro OTC	N-acetiltirosina	2307037	40	20230915*
Euro OTC	N-acetiltirosina	2307037	20	20230915*
EDQM	Nitrato de isoconazol	1.1	40	CRS
Caelo	Nitrato de potássio	12236703	40	20120807
Caelo	Nitrato de prata	181276	40	20180716*
EDQM	Nitrato de sertaconazol	2.0	26	CRS
Caelo	Nitrato de sódio	11045910	40	20110225
Fagron	Nitrato de tiamina	15A30-B06-309069	60	AR-16-FG-005855-01
Caelo	Nitrito de sódio	171360	30	20170522*
Caelo	Noz moscada	12067304	40	20120320
Caelo	Noz moscada	13266002	40	20130906
Caelo	Noz moscada	22002543003	30	20221004
Klenk	Noz moscada	7320A121002	40	20121012
Caelo	Olíbano	12120005	40	1402495
Caelo	Olíbano	13112801	40	20130503
Fagron	Ondansetrona cloridrato dihidratado	24H07-H03-00987	40	20240808
Fagron	Ondansetrona cloridrato dihidratado	24H07-H03-00987	20	20240808
Euro OTC	Orotato de cálcio dihidratado	1009035-01	40	20101019
Euro OTC	Orotato de cálcio dihidratado	1411003	40	20160331*
Fagron	Orotato de cálcio dihidratado	16F13-B04-324144	40	20161108
Euro OTC	Orotato de cobre dihidratado	1901040-01	50	20190319
Euro OTC	Orotato de cobre dihidratado	2203016	40	20220520*
Euro OTC	Orotato de cobre dihidratado	2203016	20	20220520*
Caelo	Óxido de cálcio	182244	39	20181106*
Caelo	Óxido de magnésio, leve	180818	40	20180322*
Euro OTC	Óxido de magnésio, pesado	1709011-02	40	20170915
Caelo	Óxido de zinco	14038101	40	20140205
EDQM	Oxitetraciclina	8.0	40	CRS
Caelo	Pau-campeche (Haematoxylum campechianum)	11074105	40	from supplier

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Pé-de-leão	12153306	40	20120618
Euro OTC	Permanganato de potássio	1708016-02	40	20170824
Caelo	Pétala de papoula, cortada	12008104	40	20120131
Caelo	Pétala de rosa vermelha	11304912	40	20111107
Fagron	Phenibut	24H26-B009	40	20240917*
Fagron	Phenibut	24H26-B009	20	20240917*
Caelo	Pimenta	12192311	40	1403490
Caelo	Pimenta	13221114	40	20130805
Caelo	Pimenta	23001971003	30	-
Caelo	Pimenta	24100075001	30	20240924
Caelo	Pimenta branca	12294902	40	1403488
Caelo	Pimenta branca	12294905	40	20121130
Caelo	Pimenta branca	14010703	40	20140122
Caelo	Pimenta-da-Jamaica pulverizada (especiaria)	12042703	40	from supplier
Caelo	Pimpinela	12027410	40	20120206
Caelo	Pimpinela	12027407	40	20120206
Caelo	Pimpinela	12024406	40	20120206
Fagron	Piroxicam	VLSPRM0022425	40	20240512*
Fagron	Piroxicam	VLSPRM0022425	20	20240512*
Sigma-Aldrich	Pivalato de prednisolona	P2805000	40	CRS
Caelo	Plantago (Plantago lanceolata)	12362902	40	20121220
Caelo	Pó de pedra-pomes	180533	40	20180222*
Caelo	Polentilha	11328105	40	20111130
Galke	Polentilha	22840	40	from supplier
Caelo	Polygonum aviculare	14079304	40	20140402
Klenk	Polygonum aviculare	4301A120912	40	20120924
Caelo	Prata coloidal	173615	40	20180312*
Caelo	Psyllium, cascas	12148103	40	20120628
Caelo	Psyllium, semente	11185807	40	20110727
Fagron	Pullulan	24H27-B078	20	20240916*
Caelo	Quercus alba	10348617	40	20101221
Caelo	Quercus alba	11351207	40	1403492
Caelo	Quercus alba	13360306	40	20131203
Kräuter Schulte	Raiz de Achyranthes bidentata, cortada	45053	40	from supplier
Caelo	Raiz de aipo, cortada	10270002	40	20101006
Caelo	Raiz de alcaçuz	12267103	40	20120917
Caelo	Raiz de alcaçuz, descascada	12227101	40	20120813
Caelo	Raiz de alcaçuz, descascada	12227106	40	20120813
Caelo	Raiz de angélica	12168701	40	pending
Caelo	Raiz de angélica	12080404	40	1403053
Caelo	Raiz de angélica	12080409	40	20120322
Klenk	Raiz de angélica	6085B120614	40	20120621
Klenk	Raiz de angélica	6085B120614	60	1509356
Caelo	Raiz de aspargo, cortada	10299010	40	pending
Caelo	Raiz de Astrantia major, cortada	12101804	60	20120405
Caelo	Raiz de Astrantia major, cortada	13341204	40	20131030
Caelo	Raiz de bardana	11100801	40	20110523
Caelo	Raiz de cálamo	12076404	40	20120328
Caelo	Raiz de cálamo, descascada	12239001	40	20120905
Caelo	Raiz de cálamo, descascada	12295902	40	20121025
Caelo	Raiz de Carlina acaulis	12163702	40	20120628
Caelo	Raiz de Carlina acaulis	12232802	40	20120822
Caelo	Raiz de elecampane, cortada	12113303	40	20120427
Klenk	Raiz de elecampane, cortada	6341B120611	40	20120620
Caelo	Raiz de fraxinela, cortada	10189103	40	20100804

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Raiz de fraxinela, cortada	11314705	40	pending
Caelo	Raiz de fraxinela, cortada	11314705	80	20111115
Caelo	Raiz de fraxinela, cortada	14110802	60	20140428
Caelo	Raiz de garra-do-diabo	12031806	40	20120222
Caelo	Raiz de garra-do-diabo	13298202	40	20130926
Caelo	Raiz de genciana	12244603	40	20120914
Caelo	Raiz de genciana, pulverizada	12007103	50	1403630
Caelo	Raiz de genciana, pulverizada	12007106	40	20120117
Caelo	Raiz de genciana, pulverizada	13410503	40	1508394
Caelo	Raiz de ginseng	12080208	40	20120329
Caelo	Raiz de ginseng	11349206	40	20111227
Caelo	Raiz de ginseng	13341008	40	20131029
Caelo	Raiz de ginseng	13237805	40	20130816
Caelo	Raiz de Ononis repens	12330001	40	20121127
Klenk	Raiz de Ononis repens	6411B130404	40	20130507
Caelo	Raiz de Orris	12206802	40	20120813
Klenk	Raiz de peônia, cortada	6421B120327	60	20120403
Caelo	Raiz de prímula, cortada	12064506	40	20120319
Caelo	Raiz de salsa	12080301	40	20120329
Caelo	Raiz de valeriana, pulverizada	12138005	40	1403809
Caelo	Raiz de valeriana, pulverizada	12138008	40	1508496
Caelo	Raiz de valeriana, pulverizada	13113204	60	pending
Caelo	Raiz de zedoária	12125301	40	20120522
Caelo	Raiz de zedoária, pulverizada	12344601	40	1403489
Caelo	Raiz de zedoária, pulverizada	13165501	40	pending
Caelo	Raiz de zedoária, pulverizada	14249001	60	20141008
Caelo	Resina Podophyllum (de Podophyllum peltatum)	12287810	40	1405242
Fagron	Resveratrol	24I18-B028	40	20241008*
Fagron	Resveratrol	24I18-B025	40	20241008*
Fagron	Resveratrol	24I18-B028	20	20241008*
Fagron	Resveratrol	24I18-B025	20	20241008*
Euro OTC	Ribavirina	1304027-01	45	AR-16-FG-007485-01
Euro OTC	Ribavirina	1308001	45	20130902*
Euro OTC	Ribavirina	1604012	40	20160428*
Euro OTC	Ribavirina	1304027-02	40	20160429
Caelo	Rifampicina	152446	40	20150831*
Caelo	Rifaximina	161053	60	20160607*
Caelo	Rizoma de galanga	12125001	40	20120516
Caelo	Rizoma de galanga	11375904	40	20120109
Caelo	Rizoma de galanga	12330305	40	1403491
Caelo	Rizoma de galanga	11375909	40	1403324
Caelo	Rizoma de galanga	12330308	40	20121203
Caelo	Rizoma de galanga	14159504	60	1511617
Caelo	Rizoma de grama-francesa, cortada	12186702	40	20120629
Klenk	Rizoma de ruscus, cortado	7081B110301	60	20130131
Caelo	Rosa canina, casca	11301407	60	20111110
Caelo	Rosa-mosqueta com casca, cortada	12064202	40	20120328

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Rosa-mosqueta com casca, cortada	11232204	40	20110919
Caelo	Ruibarbo	12211906	40	20120827
Caelo	Ruibarbo	13235213	40	20130822
Caelo	Ruibarbo, pulverizado	11043818	60	1403280
Caelo	Ruibarbo, pulverizado	16009901	60	9886
Fagron	Rutosídeo tri-hidratado	13K12-B06-295483	60	20131204
Caelo	Sabugueiro	12221902	40	20120821
Fagron	s-acetilglutationa	22G01-B02-225858	40	20220706
Fagron	s-acetilglutationa	23D21-B10-229486	40	20230809
Fagron	s-acetilglutationa	22G01-B02-225858	20	20220706
Fagron	s-acetilglutationa	23D21-B10-229486	20	20230809
Caelo	Sal térmico artificial a	181633	40	20180621*
Klenk	Salsa, esfregada	4262A091116	60	20110719
Caelo	Salsaparrilha, cortada	10230402	60	20100909
Caelo	Semente de abóbora	12249002	40	1404542
Caelo	Semente de abóbora	12249006	40	20120917
Caelo	Semente de alfarroba pulverizado	10376516	40	20110106
Caelo	Semente de alfarroba pulverizado	13379403	40	from supplier
Caelo	Semente de cominho preto	11233503	40	1403495
Caelo	Semente de mostarda preta, pulverizada	13358304	40	pending
Caelo	Semente de mostarda preta, pulverizada	16051807	60	9887
Klenk	Semente de mostarda preta, pulverizada	7434A120712	40	AR-15-FG-006711-01
Caelo	Semente de mostarda, preta	12189303	40	1403472
Caelo	Semente de mostarda, preta	15120405	60	AR-17-FG-007964-01
Caelo	Semente de mostarda, preta	23000940006	30	20230523
Caelo	Semente de psílio	10291206	40	pending
Caelo	Semente de psílio	10291205	80	20101119
Caelo	Semente de psílio	13305903	40	pending
Klenk	Semente de rosa mosqueta	7240A120402	60	20120404
Klenk	Semente de trigo sarraceno	7510A111011	40	from supplier
Klenk	Semente de trigo sarraceno	7510A111011	60	pending
Caelo	Semente de urtiga	12131507	40	1402203
Caelo	Semente de urtiga	11126211	40	pending
Caelo	Semente de urtiga	13387110	40	1410300
Klenk	Semente de urtiga	7470A111117	40	pending
Klenk	Semente de urtiga	7470A221024-02	30	20221122
Caelo	Sempre-viva	11293101	40	20111028
Caelo	Sequoia africana, cortada	12049604	40	20120229
Caelo	Sílica coloidal anidra	181124	40	20180424*
Sigma-Aldrich	Silicato de alumínio e sódio	102527683	40	not required
Caelo	Sinapis alba, semente	13064301	40	pending
Caelo	Sinapis alba, semente	13380501	40	20140103
Fagron	Sinvastatina	24D29-B07-002224	40	20240730
Fagron	Sinvastatina	24H01-B12-002225	40	20240927
Fagron	Sinvastatina	24D29-B07-002224	20	20240730
Fagron	Sinvastatina	24H01-B12-002225	20	20240927
Caelo	Sódio 4-hidroxibenzoato de metila	15358708	40	AR-16-FG-015095-01
Caelo	Sódio 4-hidroxibenzoato de metila	15358708	40	20151127
Caelo	Sódio 4-hidroxibenzoato de metila	15358709	40	20151127
Caelo	Sódio 4-hidroxibenzoato de metila	15358713	40	20151127

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Sódio 4-hidroxibenzoato de metila	170519	40	20170308*
Caelo	Sódio 4-hidroxibenzoato de metila	191439	40	20190628*
Caelo	Softisan® 601	13296104	40	1403144
Caelo	Softisan® 601	14099604	40	1504720
Caelo	Softisan® 601	15184905	60	20150611
Caelo	Softisan® 601	162364	40	20160823*
Caelo	Softisan® 601	162364	40	20160823*
Caelo	Softisan® 601	172178	40	20170817*
Caelo	Softisan® 601	20003054001	40	20201001
Caelo	Stellaria media, cortada	13040502	40	1403482
Caelo	Stellaria media, cortada	13254411	40	1412550
USP	Succinato de metoprolol	R11100	40	CRS
Caelo	Sulfamerazina	10218403	30	20100914
Fagron	Sulfametoxazol	22H23-B16-225919	40	20220909
Fagron	Sulfametoxazol	22H23-B16-225919	20	20220909
Fagron	Sulfato de 8-quinolinol monoidratado	12H21-N08	40	20120831
Caelo	Sulfato de bário	171113	40	20170509*
Caelo	Sulfato de cálcio di-hidratado	163363	40	20161214*
Caelo	Sulfato de cálcio hemi-hidratado	153451	30	20151103*
Caelo	Sulfato de cobre (II) penta-hidratado	162409	40	20160825*
Caelo	Sulfato de ferro (II) hepta-hidratado	11340509	40	1401568
Caelo	Sulfato de ferro (III) hidratado	170991	40	20170523*
Caelo	Sulfato de hidroxicloroquina	20001292	40	20200427*
Caelo	Sulfato de magnésio seco	172990	40	20171129*
Caelo	Sulfato de morfina	12153212	40	0914F-07776
Caelo	Sulfato de morfina	11333103	40	0914E-07776
Caelo	Sulfato de morfina	15255703	60	1416Q-07776
Caelo	Sulfato de morfina	15295802	40	1917R-07776
Caelo	Sulfato de morfina	17331510	40	2319I-07776
Caelo	Sulfato de morfina	12153212	60	0914F-07776
Caelo	Sulfato de morfina	11333103	60	0914E-07776
Caelo	Sulfato de morfina	15255703	60	1416Q-07776
Caelo	Sulfato de morfina	15295802	40	1917R-07776
Caelo	Sulfato de morfina	17331510	40	2319I-07776
Fagron	Sulfato de morfina	13J07-N04	40	0914G-07776
Fagron	Sulfato de morfina	14F02-B06-315405	40	1917Q-07776
Fagron	Sulfato de morfina	13J07-N04	60	0914G-07776
Fagron	Sulfato de morfina	14F02-B06-315405	40	1917Q-07776
Caelo	Sulfato de quinolinol sulfato de potássio	13071104	40	1403095
Caelo	Sulfato de quinolinol sulfato de potássio	13403501	60	20131218
Caelo	Sulfato de quinolinol sulfato de potássio	15147704	40	20150618
Caelo	Sulfato de quinolinol sulfato de potássio	15147704	40	20150618
Caelo	Sulfato de quinolinol sulfato de potássio	162218	40	20160808*
Caelo	Sulfato de quinolinol sulfato de potássio	16221809	40	20160808
Euro OTC	Sulfato de sódio, anidro	1801046-01	40	20180202

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	SyrSpend® SF Alka	15H11-B04-311722	40	1608351
Fagron	SyrSpend® SF Alka	15H11-B04-311722	40	20150902
Fagron	SyrSpend® SF Alka	15H11-B04-311722	40	1701054
Fagron	SyrSpend® SF Alka	17F14-B02-335945	20	1804106
Fagron	SyrSpend® SF Alka	15H11-B04-311722	40	20150902
Fagron	SyrSpend® SF Alka	22B04-F07-381936	40	20220317
Fagron	SyrSpend® SF Alka	22K18-F04-38394	40	20221223
Fagron	SyrSpend® SF Alka	22B04-F07-381936	20	20220317
Fagron	SyrSpend® SF Alka	22K18-F04-38394	20	20221223
Fagron	SyrSpend® SF Alka	23B16-F01-384773	20	20230502
Fagron	SyrSpend® SF pH4	15H13-B03-314611	40	20150903
Fagron	SyrSpend® SF pH4	15H13-B03-314611	40	20150903
Fagron	SyrSpend® SF pH4	16J10-B03-330757	40	20170317
Fagron	SyrSpend® SF pH4	23B13-F02-384539	40	20230403
Fagron	SyrSpend® SF pH4	23B13-F02-384539	20	20230403
Fagron	SyrSpend® SF pH4	23H11-F02-385247	20	20231005
Fagron	SyrSpend® SF pH4 neo	22B04-F01-381138	40	20220204
Fagron	SyrSpend® SF pH4 neo	23L01-H01-00941	40	20231211
Fagron	SyrSpend® SF pH4 neo	24A09-H07-00941	40	20240117
Fagron	SyrSpend® SF pH4 neo	22B04-F01-381138	10	20220204
Fagron	SyrSpend® SF pH4 neo	23K02-H08-00941	20	20231113
Caelo	Talco	22002768	40	20220928*
Euro OTC	Talco	2204002	40	20220511*
Otto Fischar	Talco	90841/1	40	from supplier
Caelo	Talidomida	13395704	60	20140207
Caelo	Talidomida	162703	40	20160929*
Caelo	Talidomida	15276711	40	1704508
Caelo	Talidomida	172100	40	20170821*
Caelo	Talidomida	182496	40	20181022*
Fagron	Talidomida	14E27B04295348	60	1503608
Fagron	Talidomida	15A13-B01-312230	40	1704509
Fagron	Tartarato de ergotamina	13H02-N01	100	20120412
Fagron	Tartarato de ergotamina	13I24-B10-288648	50	20131024
Fagron	Tartarato de ergotamina	13I24-B10-288650	60	20131024
Fagron	Tartarato de ergotamina	15B16-B05-308418	45	9384
Fagron	Tartarato de ergotamina	15B16-B05-308417	40	20150302
Fagron	Tartarato de ergotamina	15B16-B05-308418	45	9384
Fagron	Tartarato de ergotamina	15B16-B05-308417	40	20150302
Caelo	Tartarato de potássio hemi-hidratado	13331101	40	1403536
Caelo	Tartarato de potássio hemi-hidratado	13331104	60	20131002
Caelo	Tartarato de potássio hemi-hidratado	15167701	60	20150608
Caelo	Tartarato de potássio hemi-hidratado	160289	60	20160405*
Caelo	Tartarato de potássio hemi-hidratado	182203	40	20180907*
Caelo	Tartarato de potássio hemi-hidratado	192911	40	20191125*
Caelo	Tartarato de potássio hemi-hidratado	193079	40	20191125*
Caelo	Tartarato de sódio e potássio tetra-hidratado	12030207	40	20120213
Caelo	Tartarato de sódio e potássio tetra-hidratado	13216605	40	1404530
Caelo	Tartarato de sódio e potássio tetra-hidratado	14376001	60	20150204

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Tartarato de sódio e potássio tetra-hidratado	15375607	40	20151030
Caelo	Tartarato de sódio e potássio tetra-hidratado	172577	40	20171128*
Caelo	Tartarato de sódio e potássio tetra-hidratado	20000750003	40	20200506
Fagron	Teacrina	24I18-B028	40	20241011*
Fagron	Teacrina	24I14-B018	40	20241011*
Fagron	Teofilina etilenodiamina	19C04-B04-363517	40	20190823
Fagron	Teofilina etilenodiamina	20J13-F05-375387	40	20201207
Caelo	Teriaga	12289307	40	1405122
Caelo	Teriaga	13407301	40	1410336
Klenk	Teriaga	13816	60	1705088
LGC Standa…	THCA-A	1457348	30	20240417
Caelo	Tiosulfato de sódio pentahidratado	181648	40	20180712*
USP	Tobramicina	M0M058	40	CRS
Bombastus	Tomilho	23005529	30	20231213
Caelo	Tomilho	11345004	60	20111213
Caelo	Tomilho	22003890005	30	20230622
Galke	Tomilho	21932	40	from supplier
Caelo	Tormentilha	12040708	40	1403487
Caelo	Tormentilha	12013103	40	1403048
Caelo	Tormentilha	12040715	40	1403710
Caelo	Tormentilha	13220502	40	1403049
Caelo	Tormentilha	14360103	60	1606520
Klenk	Tormentilha	6914B120112	40	20120118
Caelo	Tragacanto	13277804	60	1507149
Caelo	Tragacanto	15085602	60	20150410
Caelo	Tragacanto	15379906	60	20151124
Caelo	Tragacanto	16110802	60	AR-17-FG-007533-01
Caelo	Tribromofenol bismuto	18144202	40	20180706
Fagron	Trimetoprima	21J11-B07-219183	40	20220125
Fagron	Trimetoprima	23B17-B03-232012	40	20230322
Fagron	Trimetoprima	21J11-B07-219183	20	20220125
Fagron	Trimetoprima	23B17-B03-232012	20	20230322
Euro OTC	Trissilicato de magnésio	1608024-01	40	20160908
Audor	Uridina	APIB1600169AU	40	20170711
Audor	Uridina	APIB160018211AU	40	20161118
Fagron	Uridina	11G07-N04	60	1402481
Fagron	Uridina	13K18-B31-288497	60	20131129
Caelo	Urtiga, raiz	11254903	40	20111121
Caelo	Urze, cortada	11011209	40	20110218
Caelo	Valeriana, raiz cortada	12033809	40	20120228
Caelo	Verbena	12187602	40	20120719
Klenk	Verbena	4651B120611	40	20121123
Caelo	Veronica officinalis	12162503	40	20120703
Fagron	Vimpocetina	20240501	40	20240512*
Fagron	Vimpocetina	20240501	20	20240512*
Caelo	Viola tricolor, erva	10291007	60	20101103
Caelo	Violeta, cortada	10292002	40	pending
Caelo	Violeta, cortada	13038703	40	1403481
Caelo	Violeta, cortada	13232103	40	20130821

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Appendix C: Additional validation samples (*Type C*)

Spectra for substances from the field which cannot be identified with this model also enter the validation. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *Apo-Ident* customers. They belong to *Type C*. The information provided by the customer regarding the manufacturer and batch number is taken over by *HiperScan GmbH* to a large extent unchecked.

The samples originate from 7451 batches. From these, 17 922 spectra were recorded. The spectra recorded on independent samples of substances from the field which can be identified with the model are listed respectively in the section *Type C* for the individual substances and do not appear again elsewhere in this list.

0 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Supplier	Substance	Batch	Spectra
Euro OTC	Ácido desoxicólico	1305051-01	1
Fagron	Ácido desoxicólico	13J21-N14	1
Gehe	Ácido desoxicólico	2012060253	1
GEHE 21.10.2014	Ácido desoxicólico	13F13-N06	1
Dr. Behr	Ácido dimercaptossuccínico	WE14020002	1
Anzag	Ácido tricloroacético	12135204	2
apomix	Ácido tricloroacético	12G04-M11	1
Caelo	Ácido tricloroacético	12135201	1
Caelo	Ácido tricloroacético	12g04m11	1
Caelo	Ácido tricloroacético	11294318	1
Caelo	Ácido tricloroacético	12135203	1
Caelo	Ácido tricloroacético	12135210	2
Caelo	Ácido tricloroacético	6091306	1
Caelo	Ácido tricloroacético	14101711	1
Caelo	Ácido tricloroacético	13056203	3
Caelo	Ácido tricloroacético	12135207	5
Caelo	Ácido tricloroacético	13056212	1
Caelo	Ácido tricloroacético	10379401	1
Caelo	Ácido tricloroacético	10130802	1
Fagron	Ácido tricloroacético	13B19-M04	1
Fagron	Ácido tricloroacético	13H22-M04	1
Merck	Ácido tricloroacético	12821	1
Caelo	Ácido tricloroacético	13056213	1
Caelo	Ácido tricloroacético	13056209	1
Fagron	Índigo-carmim	12K06-N11	1
Fagron	Índigo-carmim	12A20-N067-16	1
Fagron	Índigo-carmim	5132316	1
Fagron	Índigo-carmim	13K12-N01	1
Fagron	Índigo-carmim	11F09-N06	1
Euro OTC	Óxido de magnésio, pesado	1205012-01	1
Euro OTC	Óxido de magnésio, pesado	1012033-01	1

A

Supplier	Substance	Batch	Spectra
Caelo	Abrótano, cortada	2091305	1
Klenk	Abrótano, cortada	21081301	1
Klenk	Abrótano, cortada	26011403	1
Nachprüfung	Abrótano, cortada	3451A070919	1
Noweda	Abrótano, cortada	3451A120312	19
Bahnhof-Apotheke	Absinto (Artemisia absinthium)	17-121107	1
Bombastus	Absinto (Artemisia absinthium)	281000	1
Bombastus	Absinto (Artemisia absinthium)	265417	2
Bombastus	Absinto (Artemisia absinthium)	221868	1
Caelo	Absinto (Artemisia absinthium)	11285802	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Absinto (Artemisia absinthium)	11285810	6
Caelo	Absinto (Artemisia absinthium)	6101203	1
Caelo	Absinto (Artemisia absinthium)	12355801	20
Caelo	Absinto (Artemisia absinthium)	7031301	1
Caelo	Absinto (Artemisia absinthium)	12355807	10
Caelo	Absinto (Artemisia absinthium)	13174401	3
Caelo	Absinto (Artemisia absinthium)	7011401	1
Caelo	Absinto (Artemisia absinthium)	13381902	3
Caelo	Absinto (Artemisia absinthium)	13381905	1
Caelo	Absinto (Artemisia absinthium)	15408304	1
Caelo	Absinto (Artemisia absinthium)	13174402	2
Caelo	Absinto (Artemisia absinthium)	11285805	2
Caelo	Absinto (Artemisia absinthium)	12355804	8
Caelo	Absinto (Artemisia absinthium)	12355802	3
Caelo	Absinto (Artemisia absinthium)	12355805	4
Caelo	Absinto (Artemisia absinthium)	12355808	2
Caelo	Absinto (Artemisia absinthium)	11285803	1
Caelo	Absinto (Artemisia absinthium)	272957	1
Caelo	Absinto (Artemisia absinthium)	277513	1
Galke	Absinto (Artemisia absinthium)	21330	1
Gehe	Absinto (Artemisia absinthium)	11285811	1
Gehe	Absinto (Artemisia absinthium)	13381901	1
Klenk	Absinto (Artemisia absinthium)	3461A121130	2
Klenk	Absinto (Artemisia absinthium)	3461A110324	2
Klenk	Absinto (Artemisia absinthium)	A110324	1
Klenk	Absinto (Artemisia absinthium)	3461A1100324	1
Phoenix	Absinto (Artemisia absinthium)	12103003	8
Phönix	Absinto (Artemisia absinthium)	12355806	7
Sanacorp	Absinto (Artemisia absinthium)	12103002	2
Caelo	Absinto (Artemisia absinthium)	12355803	27
Klenk	Açafrão (Crocus sativus)	384A110608	1
Klenk	Açafrão (Crocus sativus)	384A-120410	1
Klenk	Açafrão (Crocus sativus)	384A130320	2
Klenk	Açafrão (Crocus sativus)	384a120410	1
Bombastus	Açafrão de java (Curcuma xa…	288629	1
Bombastus	Açafrão de java (Curcuma xa…	262792	1
Bombastus	Açafrão de java (Curcuma xa…	277130	1
Bombastus	Açafrão de java (Curcuma xa…	282221	2
Bombastus	Açafrão de java (Curcuma xa…	28221	1
Bombastus	Açafrão de java (Curcuma xa…	284242	2
Caelo	Açafrão de java (Curcuma xa…	25041313	1
Caelo	Açafrão de java (Curcuma xa…	12319201	1
Caelo	Açafrão de java (Curcuma xa…	13262907	1
Caelo	Açafrão de java (Curcuma xa…	14309503	1
Caelo	Açafrão de java (Curcuma xa…	15120202	3
Caelo	Açafrão de java (Curcuma xa…	16094101	1
Caelo	Açafrão de java (Curcuma xa…	14017706	1
Caelo	Açafrão de java (Curcuma xa…	11182903	1
Caelo	Açafrão de java (Curcuma xa…	17042002	1
Caelo	Açafrão de java (Curcuma xa…	12319206	2
Caelo	Açafrão de java (Curcuma xa…	17042003	1
Caelo	Açafrão de java (Curcuma xa…	12319206	2
Galke	Açafrão de java (Curcuma xa…	15540	1
Galke	Açafrão de java (Curcuma xa…	15540	1
Klenk	Açafrão de java (Curcuma xa…	6731B160426	1
Kenk / Phoenix	Açafrão de java (Curcuma xa…	6731B130117	1
Klenk	Açafrão de java (Curcuma xa…	B130117	1
Klenk	Açafrão de java (Curcuma xa…	6731B150630	1
Noweda	Açafrão de java (Curcuma xa…	6731B180412	1
Caelo	Açafrão em fios	10184811	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Açafrão em fios	11071310	1
Caelo	Açafrão em fios	15101305	1
Caelo	Açafrão em fios	21011403	1
Caelo	Açafrão em fios	12108311	2
Caelo	Açafrão em fios	10184822	1
Caelo	Açafrão em fios	12108308	2
Fagron	Açafrão em fios	380A120416	1
Klenk	Açafrão em fios	380A130613	1
Caelo	Agarikon (Laricifomes offic...	11024502	1
Caelo	Agrião (Nasturtium officina...	12031602	1
Caelo	Agrião (Nasturtium officina...	12031601	1
Caelo	Agrião (Nasturtium officina...	12031606	1
Caelo	Agrião (Nasturtium officina...	12031603	1
Caelo	Agrião (Nasturtium officina...	12031604	2
Caelo	Agrião (Nasturtium officina...	13104401	4
Caelo	Agrião (Nasturtium officina...	107063	1
Caelo	Agrião (Nasturtium officina...	12031605	1
Caelo	Agrião (Nasturtium officina...	13104402	2
Caelo	Agrião (Nasturtium officina...	13104404	2
Caelo	Agrião (Nasturtium officina...	13104405	1
Caelo	Agrião (Nasturtium officina...	13104403	5
Caelo	Agrião (Nasturtium officina...	13104406	1
Alliance	Agrimônia (Agrimonia eupatoria)	11374004	5
Anzag 05.12.12	Agrimônia (Agrimonia eupatoria)	11374002	3
Caelo	Agrimônia (Agrimonia eupatoria)	10325502	2
Caelo	Agrimônia (Agrimonia eupatoria)	10325505	1
Caelo	Agrimônia (Agrimonia eupatoria)	12382903	1
Caelo	Agrimônia (Agrimonia eupatoria)	1137407	1
Caelo	Agrimônia (Agrimonia eupatoria)	11374005	2
Caelo	Agrimônia (Agrimonia eupatoria)	12382901	3
Caelo	Agrimônia (Agrimonia eupatoria)	3481-A-110324	1
Caelo	Agrimônia (Agrimonia eupatoria)	11374006	6
Celo	Agrimônia (Agrimonia eupatoria)	11374003	1
Galke	Agrimônia (Agrimonia eupatoria)	2002	1
Herbasinica	Agrimônia (Agrimonia eupatoria)	11374007	1
Klenk	Agrimônia (Agrimonia eupatoria)	3481C120508	1
Noweda	Agrimônia (Agrimonia eupatoria)	9300106	1
Noweda	Agrimônia (Agrimonia eupatoria)	10325503	2
Sino Phyto	Agrimônia (Agrimonia eupatoria)	12382905	5
Bombastus	Alcachofra (Cynara scolymus...	8202213593	1
Caelo	Alcachofra (Cynara scolymus...	12173302	3
Caelo	Alcachofra (Cynara scolymus...	12173304	3
Caelo	Alcachofra (Cynara scolymus...	12173307	6
Caelo	Alcachofra (Cynara scolymus...	2312I-03593	1
Caelo	Alcachofra (Cynara scolymus...	12173306	2
Caelo	Alcachofra (Cynara scolymus...	13037607	4
Caelo	Alcachofra (Cynara scolymus...	13037608	1
Caelo	Alcachofra (Cynara scolymus...	13037603	1
Caelo	Alcachofra (Cynara scolymus...	81232298	1
Caelo	Alcachofra (Cynara scolymus...	12173307-3260315072	1
Caelo	Alcachofra (Cynara scolymus...	13310706	1
Kenk / Phoenix	Alcachofra (Cynara scolymus...	1981B130111	3
Klenk	Alcachofra (Cynara scolymus...	B121025	2
Klenk	Alcachofra (Cynara scolymus...	1981B121025	2
Klenk	Alcachofra (Cynara scolymus...	1981B120413	1
Alfred Galke	Alcarávia	20069	1
Anzag ek: 2,59EUR 19...	Alcarávia	11003216	3
Caelo	Alcarávia	12226609	5
Bahnhof-Apotheke	Alcarávia	18-120709	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Alcarávia	275849	1
Bombastus	Alcarávia	282269	1
Bombastus	Alcarávia	270124	1
Caelo	Alcarávia	12226603	7
Caelo	Alcarávia	12226606	2
Caelo	Alcarávia	12226504	1
Caelo	Alcarávia	11003207	1
Caelo	Alcarávia	27121202	1
Caelo	Alcarávia	12343403	1
Caelo	Alcarávia	11003211	1
Caelo	Alcarávia	2103311537	1
Caelo	Alcarávia	12226601	1
Caelo	Alcarávia	4061303	1
Caelo	Alcarávia	11378309	1
Caelo	Alcarávia	413M	1
Caelo	Alcarávia	12226614	2
Caelo	Alcarávia	1226608	1
Caelo	Alcarávia	13306003	1
Caelo	Alcarávia	13397102	2
Caelo	Alcarávia	13397104	2
Caelo	Alcarávia	13091401	1
Caelo	Alcarávia	13306004	1
Caelo	Alcarávia	13306005	2
Caelo	Alcarávia	13306006	4
Caelo	Alcarávia	13306008	2
Caelo	Alcarávia	15097109	3
Caelo	Alcarávia	15097110	1
Caelo	Alcarávia	16308502	1
Caelo	Alcarávia	16165308	1
Caelo	Alcarávia	15409105	1
Caelo	Alcarávia	13306001	1
Caelo	Alcarávia	24659273	1
Caelo	Alcarávia	11121704	1
Caelo	Alcarávia	18121717	1
Caelo	Alcarávia	16308504	1
Caelo	Alcarávia	11003217	5
Caelo	Alcarávia	15409102	4
Caelo	Alcarávia	12226611	3
Caelo	Alcarávia	13306007	4
Caelo	Alcarávia	15097101	8
Caelo	Alcarávia	16308506	2
Caelo	Alcarávia	15097102	1
Caelo	Alcarávia	1509101	1
Caelo	Alcarávia	13397105	8
Caelo	Alcarávia	15097103	5
Caelo	Alcarávia	290416	1
Caelo	Alcarávia	15097115	6
Caelo	Alcarávia	15409101	1
Caelo	Alcarávia	12226501	5
Caelo	Alcarávia	9267815	1
Caelo	Alcarávia	811E-01537	1
Caelo	Alcarávia	15097002	1
Caelo	Alcarávia	17256303	2
Caelo	Alcarávia	15097111	3
Caelo	Alcarávia	15097116	1
Caelo	Alcarávia	15409104	3
Caelo	Alcarávia	18303903	1
Caelo	Alcarávia	13306002	5
Caelo	Alcarávia	15097108	4
Caelo	Alcarávia	15409103	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alcarávia	16308501	2
Caelo	Alcarávia	17256304	1
Caelo	Alcarávia	18009206	1
Caelo	Alcarávia	12226612	8
Caelo	Alcarávia	15097107	2
Caeol/Phönix	Alcarávia	16308503	5
Caesar & Loretz Gm...	Alcarávia	9267824	2
Caesar & Loretz Gm...	Alcarávia	11003213	2
Caesar & Loretz/Noweda	Alcarávia	15056601	1
Galke	Alcarávia	21257	1
Galke	Alcarávia	23627	1
Galke	Alcarávia	27450	1
GALKE	Alcarávia	30030	1
Klenk	Alcarávia	2770A130910	1
Hepart AG	Alcarávia	B-224,kbA	1
Caelo	Alcarávia	12226608	4
Caelo	Alcarávia	1222608	1
Klenk	Alcarávia	2770A110601	9
Klenk	Alcarávia	2770A110818	8
Klenk	Alcarávia	1810A-01537	1
Klenk	Alcarávia	A120905	3
Klenk	Alcarávia	2770A130521	12
Klenk	Alcarávia	2270A130521	1
Klenk	Alcarávia	412091-1-P	1
Klenk	Alcarávia	2770A131008	2
Klenk	Alcarávia	2820A150713	1
Klenk	Alcarávia	2770A120403	14
Klenk	Alcarávia	2770a120905	2
Klenk	Alcarávia	5213A1537	1
Klenk	Alcarávia	2770A140708	6
Klenk	Alcarávia	2770A160304	2
Noweda	Alcarávia	12226503	7
Noweda	Alcarávia	12226605	3
Noweda	Alcarávia	299573	2
Caelo	Alcarávia	13041903	1
Caelo	Alcarávia	15097118	1
Caelo	Alcarávia	2041017/16308501	1
sanacorp	Alcarávia	2656259	1
Sanacorp	Alcarávia	2770A120905	4
Sanacorp	Alcarávia		2
Caelo	Alcarávia	15097117	1
Caelo	Alcarávia	12226604	5
Caelo	Alcarávia	13041901	1
Wolf	Alcarávia	B-224	1
Euro OTC	Alginato de sódio	1509036-01	1
Fagron	Alginato de sódio	14G22-B99	1
phönix	Alginato de sódio	11509036-02	1
Caelo	Aloés, cabo	12232102	1
Caelo	Aloés, cabo	505125	1
Caelo	Aloés, cabo	12338206	2
Caelo	Aloés, cabo	25111303	1
Caelo	Aloés, cabo	12338209	1
Caelo	Aloés, cabo	11041402	1
Caelo	Aloés, cabo	11061406	1
Caelo	Aloés, cabo	25071402	1
Caelo	Aloés, cabo	15283006	1
Caelo	Aloés, cabo	16202404	2
Caelo	Aloés, cabo	16202407	1
Caelo	Aloés, cabo	16202403	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Aloés, cabo	15283001	1
Caelo	Aloés, cabo	12338201	4
Caelo	Aloés, cabo	15283010	2
Caelo	Aloés, cabo	16202401	2
Caelo	Aloés, cabo	12338203	4
Caesar/Noweda	Aloés, cabo	2013E-01089	1
Caesar/Noweda	Aloés, cabo	12338211	1
Gehe	Aloés, cabo	18235801	1
phönix	Aloés, cabo	15283011	2
Caelo	Aloés, cabo	15283007	1
Caelo	Aloés, cabo	16202406	2
Klenk	Amêndoas amargas, inteiras	40A161028	13
Klenk	Amêndoas amargas, inteiras	40A-150904	2
Klenk	Amêndoas amargas, inteiras	40A161206	8
Apotheke Bühlau	Amêndoas amargas, inteiras	267467	2
Bombastus	Amêndoas amargas, inteiras	275001	3
Bombastus	Amêndoas amargas, inteiras	275600	1
Bombastus	Amêndoas amargas, inteiras	283369	1
Bombastus	Amêndoas amargas, inteiras	284978	1
Bombastus	Amêndoas amargas, inteiras	297921	1
Bombastus	Amêndoas amargas, inteiras	304961	1
Bombastus	Amêndoas amargas, inteiras	1700352	2
Bombastus	Amêndoas amargas, inteiras	17000353	1
Bombastus	Amêndoas amargas, inteiras	306048	1
Bombastus	Amêndoas amargas, inteiras	303218	2
Bombastus	Amêndoas amargas, inteiras	305322	2
Bombastus	Amêndoas amargas, inteiras	275601	1
Bombastus	Amêndoas amargas, inteiras	267529	1
Caelo	Amêndoas amargas, inteiras	12239604	1
Caelo	Amêndoas amargas, inteiras	13242001	1
Caelo	Amêndoas amargas, inteiras	5121301	1
Caelo	Amêndoas amargas, inteiras	15193103	1
Euro OTC	Amêndoas amargas, inteiras	290973	2
Fagron	Amêndoas amargas, inteiras	40A161005	5
Caelo	Amêndoas amargas, inteiras	16221202	1
Klenk	Amêndoas amargas, inteiras	40A150904	18
Klenk	Amêndoas amargas, inteiras	40A120924	4
Klenk	Amêndoas amargas, inteiras	40A121010	11
Klenk	Amêndoas amargas, inteiras	40A111004	1
Klenk	Amêndoas amargas, inteiras	40A111117	7
Klenk	Amêndoas amargas, inteiras	40A140908	19
Klenk	Amêndoas amargas, inteiras	40A0130909	1
Klenk	Amêndoas amargas, inteiras	40A130909	9
Klenk	Amêndoas amargas, inteiras	40A150905	1
Klenk	Amêndoas amargas, inteiras	40A0161005	1
AHD 10.02.17 EK.3,50	Anis	16200801	5
Anzag 06.04.2016	Anis	15398601	1
Caelo	Anis	1137033	1
Aurica	Anis	521302895	1
Bahnhof-Apotheke	Anis	7-120913	1
Berkel AHK	Anis	11374103	1
Berkel AHK	Anis	14194401	1
Bombastus	Anis	285778	2
Bombastus	Anis	309836	1
Bombastus	Anis	282917	2
Bombastus	Anis	289846	2
Bombastus	Anis	285777	1
Bombastus	Anis	305177	1
Caelo	Anis	13037805	11
Caelo	Anis	PrüfNr4913E-01530	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Anis	13333913	1
Caelo	Anis	11101202	3
Caelo	Anis	10081207	1
Caelo	Anis	11101201	1
Caelo	Anis	11101215	3
Caelo	Anis	11370303	13
Caelo	Anis	10247202	1
Caelo	Anis	4061301	1
Caelo	Anis	5061301	1
Caelo	Anis	13037804	7
Caelo	Anis	13037801	1
Caelo	Anis	5091304	1
Caelo	Anis	13037901	1
Caelo	Anis	12360801	1
Caelo	Anis	13037808	9
Caelo	Anis	13333903	4
Caelo	Anis	13333901	6
Caelo	Anis	13333902	9
Caelo	Anis	5121401	1
Caelo	Anis	13333906	3
Caelo	Anis	13333909	2
Caelo	Anis	13333910	4
Caelo	Anis	13333914	1
Caelo	Anis	13333916	1
Caelo	Anis	15046103	3
Caelo	Anis	15046106	1
Caelo	Anis	15049103	1
Caelo	Anis	16165303	1
Caelo	Anis	16165304	4
Caelo	Anis	16165302	1
Caelo	Anis	15398607	1
Caelo	Anis	161635305	1
Caelo	Anis	17045603	3
Caelo	Anis	17045601	1
Caelo	Anis	16165308	1
Caelo	Anis	17045609	4
Caelo	Anis	17045611	3
Caelo	Anis	11121705	1
Caelo	Anis	13037803	2
Caelo	Anis	13037809	12
Caelo	Anis	17045602	3
Caelo	Anis	15398605	7
Caelo	Anis	15046102	12
Caelo	Anis	111101213	1
Caelo	Anis	11101213	2
Caelo	Anis	15046101	5
Caelo	Anis	3314E-01530	1
Caelo	Anis	2215M-01530	1
Caelo	Anis	2916E-01530	1
Caelo	Anis	15283201	6
Caelo	Anis	11370301	10
Caelo	Anis	13333908	7
Caelo	Anis	11370308	3
Caelo	Anis	15398603	5
Caelo	Anis	16165306	5
Caelo	Anis		1
Caelo	Anis	11101203	6
Caelo	Anis	13037807	2
Caelo	Anis	11370302	4
Caelo	Anis	12226402	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Anis	140913a	1
Caelo	Anis	13333907	4
Caelo	Anis	1539805	1
Caelo	Anis	17045608	1
Caelo	Anis	15046109	5
Caelo	Anis	15046110	1
Caelo	Anis	13037808-3560412014	1
Caelo	Anis	16165305	6
Caelo	Anis	15398601I-301216/5	1
Caelo	Anis	15398602	5
Caelo	Anis	13333912	3
Caesar & Loretz/Noweda	Anis	153986002	1
Fagron	Anis	11370304	7
galke	Anis	19654	1
Galke	Anis	21278	1
Galke	Anis	22274	1
Galke	Anis	23464	1
GALKE	Anis	29047	1
Gehe	Anis	10247203	1
Gutenberg-Apotheke	Anis	1333902	1
Hepart AG	Anis	B216346,kbA	1
Jenne	Anis	2700A131015	2
Klenk	Anis	212M-01530	1
Klenk	Anis	2700A110701	7
Klenk	Anis	2901311530	1
Klenk	Anis	2103311530	1
Klenk	Anis	3113Q01530	1
Klenk	Anis	2700A130527	15
Klenk	Anis	2700A160511	8
Klenk	Anis	2700A150810	2
Klenk	Anis	2700A170803	1
Klenk	Anis	2700A190107	1
Klenk	Anis	2700A-110701	1
Klenk	Anis	2700A120320	8
Klenk	Anis	2700a120320	1
Klenk	Anis	2700A150901	3
Klenk	Anis	2700A12107	1
Klenk	Anis	814Q01530	1
Klenk	Anis	Klenk2700A131015	1
Klenk	Anis	2700A140129	9
Klenk	Anis	2700A121107	1
Klenk	Anis	2700A150601	11
nachprüfung	Anis	C1246	1
Nachprüfung	Anis	5010U-01530	1
Caelo	Anis	13037802	9
Caelo	Anis	11101214	6
siehe Protokoll	Anis	sieheProtokoll	1
Wolf	Anis	215346	1
Wolf	Anis	B216346	14
Wolf	Anis	216346	1
Wolf	Anis	B-671	2
Wolf	Anis	B671	1
Wolf	Anis	L401F292b	4
Wolf	Anis	L401F1413	1
Caelo	Anis estrelado	10169101	1
Caelo	Anis estrelado	10376403	2
Caelo	Anis estrelado	11314104	1
Caelo	Anis estrelado	12226211	1
Caelo	Anis estrelado	10376405	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Anis estrelado	11314103	1
Klenk	Anis estrelado	2690A101026	1
Klenk	Anis estrelado	2690A111013	3
Klenk	Anis estrelado	2696B111109	1
Klenk	Anis estrelado	B111109	1
Klenk	Anis estrelado	2690A120809	1
Klenk	Anis estrelado	2690A130903	2
Caelo	Anis estrelado, cortado	16253201	2
Caelo	Anis, esmagado	12111304	1
Caelo	Anis, esmagado	11242003	1
Caelo	Anis, esmagado	4041302	1
Caelo	Anis, esmagado	23041303	1
Caelo	Anis, esmagado	15149702	1
Caelo	Anis, esmagado	1314990	1
Caelo	Anis, esmagado	12111303	3
Gahlke	Anis, esmagado	21401	1
Gehe	Anis, esmagado	13149903	1
Caelo	Anis, esmagado	13149902	1
Caelo	Anis, esmagado	12360803	2
Klenk	Anis, esmagado	2706B100120	1
Aurica Naturheilmi...	Anis, pulverizado	521405796	1
Klenk	Anis, pulverizado	2704B110824	1
vedono	Anis, pulverizado	11306208	1
Caelo	Arruda caprária, cortada	11307903	1
Caelo	Arruda caprária, cortada	11175104	1
Caelo	Arruda caprária, cortada	11307901	1
Caelo	Arruda caprária, cortada	12017907	3
Caelo	Arruda caprária, cortada	12017914	1
Caelo	Arruda caprária, cortada	12017913	2
Caelo	Arruda caprária, cortada	12343303	6
Caelo	Arruda caprária, cortada	12343302	4
Caelo	Arruda caprária, cortada	5122013e	1
Caelo	Arruda caprária, cortada	12343305	3
Caelo	Arruda caprária, cortada	12343308	1
Galke	Arruda caprária, cortada	8378	2
Klenk	Arruda caprária, cortada	3901C110905	1
Klenk	Arruda caprária, cortada	3901B140801	1
Caelo	Arruda caprária, cortada	12017912	1
Sanacorp	Arruda caprária, cortada	12017911	1
Caelo	Arruda, cortada		1
Caelo	Arruda, cortada	9336802	1
Caelo	Arruda, cortada	12148804	1
Caelo	Arruda, cortada	12148806	1
Caelo	Arruda, cortada	12148801	1
Caelo	Arruda, cortada	11371803	1
Caelo	Arruda, cortada	12148803	2
Gehe	Arruda, cortada	12148802	1
Klenk	Arruda, cortada	A120207	1
Klenk	Arruda, cortada	4361A120207	1
Klenk	Arruda, cortada	4361A07020601	1
Klenk	Arruda, cortada	4361A100707	3
AHD	Artemísia-vulgar	521603580	1
AHD	Artemísia-vulgar	16310701	1
Caelo	Artemísia-vulgar	12016708	5
Aurica	Artemísia-vulgar	521305386	1
Caelo	Artemísia-vulgar	12016702	1
Caelo	Artemísia-vulgar	3591A110119	4
Caelo	Artemísia-vulgar	12016705	5
Caelo	Artemísia-vulgar	12016707	3
Caelo	Artemísia-vulgar	18031302	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Artemísia-vulgar	1081301	1
Caelo	Artemísia-vulgar	12382702	12
Caelo	Artemísia-vulgar	12382705	2
Caelo	Artemísia-vulgar	12382706	1
Caelo	Artemísia-vulgar	14360605	1
Caelo	Artemísia-vulgar	12016709	2
Caelo	Artemísia-vulgar	12016711	3
Caelo	Artemísia-vulgar	12382701	7
Caelo	Artemísia-vulgar	9355403	1
Galke	Artemísia-vulgar	21637	1
Caelo	Artemísia-vulgar	10355329	1
Caelo	Artemísia-vulgar	1238701	1
Klenk	Artemísia-vulgar	3591A120123	8
Klenk	Artemísia-vulgar	A120123	2
Klenk	Artemísia-vulgar	3591A130218	10
Klenk	Artemísia-vulgar	3591a130218	2
Klenk	Artemísia-vulgar	3591a120123	1
Klenk	Artemísia-vulgar	2591A130218	1
Klenk	Artemísia-vulgar	3591A11119	1
Richter	Artemísia-vulgar	b200112	1
Fagron	Aspartato de magnésio di-hi…	17C21-B05-333111	1
Klenk	Asplenium scolopendrium, cortada	4451B091116	1
Klenk	Asplenium scolopendrium, cortada	4451B120605	1
Caelo	Aveia, palha	11280008	2
Caelo	Aveia, palha	11280014	1
Caelo	Aveia, palha	11280012	2
Caelo	Aveia, palha	11280015	3
Caelo	Aveia, palha	11280017	2
Noweda	Aveia, palha	11280003	1
Caelo	Azedinha, cortada	130546	1
Gahlke	Azedinha, cortada	21479	1
Caelo	Azedinha, cortada	13289502	2
Kräuter-Schulte	Azedinha, cortada	55272	1

B

Supplier	Substance	Batch	Spectra
Anzag 22.03.13 ek:…	Babosa da montanha, pulverizada	12232102	1
Caelo	Babosa da montanha, pulverizada	11132115	1
Caelo	Babosa da montanha, pulverizada	12183007	1
Caelo	Babosa da montanha, pulverizada	12183009	3
Caelo	Babosa da montanha, pulverizada	14065905	1
Caelo	Babosa da montanha, pulverizada	15206501	1
Caelo	Babosa da montanha, pulverizada	12183008	1
Caelo	Babosa da montanha, pulverizada	12183001	1
Caelo	Babosa da montanha, pulverizada	14065906	1
Caelo	Babosa da montanha, pulverizada	11132116	2
Caelo	Babosa da montanha, pulverizada	15206514	1
Caelo	Babosa da montanha, pulverizada	15206516	1
Caelo	Babosa da montanha, pulverizada	11132116	1
Caelo	Babosa da montanha, pulverizada	12183013	3
Caesar / Gehe	Babosa da montanha, pulverizada	15206507	2
Klenk	Babosa da montanha, pulverizada	24A160620	1
Caelo	Babosa da montanha, pulverizada	16202410	1
Aurica / 11	Bagas de zimbro	521301390	1
Aurica/Phönix	Bagas de zimbro	521006043	1
Caelo	Bagas de zimbro	12028610	1
Caelo	Bagas de zimbro	12330505	2
Klenk	Bagas de zimbro	2890A101201	5
Klenk	Bagas de zimbro	2890A120709	14
Klenk	Bagas de zimbro	A120709	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Bagas de zimbro	2890a101201	3
Klenk	Bagas de zimbro	2890a120709	1
Klenk	Bagas de zimbro	2890A130513	2
Phoenix	Bagas de zimbro		1
Phönix	Bagas de zimbro	13020903	1
Sanacorp	Bagas de zimbro	12330509	1
Caelo	Bagas de zimbro, esmagado	13031302	1
Caelo	Bagas de zimbro, esmagado	14149502	1
Caelo	Bagas de zimbro, esmagado	13367302	1
Gehe	Bagas de zimbro, esmagado	13020903	1
Gehe am 27.03.2014	Bagas de zimbro, esmagado	2890A130513	1
Klenk	Bagas de zimbro, esmagado	2896B121016	7
Caelo	Bentonita	fürHerrSalloch	1
Caelo	Bentonita	1307016-01	1
Caelo	Bentonita	1311014-01	1
Clariant - Mindel-Food	Bentonita	1301	1
Noweda	Bentonita	11304415	1
Bombastus	Betônia (Stachys officinali…	12007205	2
Caelo	Betônia (Stachys officinali…	12007208	1
Caelo	Betônia (Stachys officinali…	13048906	1
Caelo	Betônia (Stachys officinali…	134048903	1
Caelo	Betônia (Stachys officinali…	13367802	1
Sanacorp	Betônia (Stachys officinali…	13048903	3
Caelo	Betônia (Stachys officinali…	12007201	1
Alliance	Bicarbonato de sódio	12324704	1
Fagron	Bicarbonato de sódio	12G11-N03	7
Anzag/ Hedinger	Bicarbonato de sódio	206027	1
Caelo	Bicarbonato de sódio	11304813	1
Caelo	Bicarbonato de sódio	8101203	1
Caelo	Bicarbonato de sódio	12132204	7
Caelo	Bicarbonato de sódio	12132219	8
Caelo	Bicarbonato de sódio	1203030-1	1
Caelo	Bicarbonato de sódio	12356303	3
Caelo	Bicarbonato de sódio	12324725	1
Caelo	Bicarbonato de sódio	12324708	1
Caelo	Bicarbonato de sódio	12356401	4
Caelo	Bicarbonato de sódio	13060117	1
Caelo	Bicarbonato de sódio	13186704	1
Caelo	Bicarbonato de sódio	12356403	1
Caelo	Bicarbonato de sódio	12356407	2
Caelo	Bicarbonato de sódio	13234004	2
Caelo	Bicarbonato de sódio	6011404	1
Caelo	Bicarbonato de sódio	13234005	4
Caelo	Bicarbonato de sódio	13234007	4
Caelo	Bicarbonato de sódio	13234202	3
Caelo	Bicarbonato de sódio	13390520	1
Caelo	Bicarbonato de sódio	13234205	1
Caelo	Bicarbonato de sódio	12132503	1
Caelo	Bicarbonato de sódio	15328602	1
Caelo	Bicarbonato de sódio	13101706	1
Caelo	Bicarbonato de sódio	11304802	2
Caelo	Bicarbonato de sódio	13186706	2
Caelo	Bicarbonato de sódio	1234702	2
Caelo	Bicarbonato de sódio	12109204	3
Caelo	Bicarbonato de sódio	13060103	8
Caelo	Bicarbonato de sódio	3012Q-01892	1
Caelo	Bicarbonato de sódio	13060120	5
Caelo	Bicarbonato de sódio	13390505	1
Caelo	Bicarbonato de sódio	13186721	1
Caelo	Bicarbonato de sódio	11304809	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bicarbonato de sódio	12132203	3
Caelo	Bicarbonato de sódio	1219204	1
Caesar & Loretz Gm…	Bicarbonato de sódio	13060102	1
Eu Rho	Bicarbonato de sódio	1203030-01	8
Euro OCT	Bicarbonato de sódio	1307017-01	1
Euro OTC	Bicarbonato de sódio	120303001	1
Euro OTC	Bicarbonato de sódio	120800801	1
Euro OTC	Bicarbonato de sódio	1012011-01	1
Euro OTC	Bicarbonato de sódio	1109029-01	8
Euro OTC	Bicarbonato de sódio	1012011	1
Euro OTC	Bicarbonato de sódio	1208008-01	9
Euro OTC	Bicarbonato de sódio	1304017-02	2
euroho/gehe	Bicarbonato de sódio	123030-02	1
Euro OTC	Bicarbonato de sódio	1104013-01	2
Euro OTC	Bicarbonato de sódio	1304017-01	5
Fagron	Bicarbonato de sódio	11K25-N05	3
Fagron	Bicarbonato de sódio	12D11-No2	1
Fagron	Bicarbonato de sódio	13D29-N09	4
Fagron	Bicarbonato de sódio	11/12-N16	1
Fagron	Bicarbonato de sódio	11I12-N16	3
Fagron	Bicarbonato de sódio	12D11-N02	9
Fagron	Bicarbonato de sódio	13G11-N03	2
Fagron	Bicarbonato de sódio	RBA3421100	3
Fagron	Bicarbonato de sódio	RBA3651200	1
Fagron	Bicarbonato de sódio	4413I01892	1
Finze	Bicarbonato de sódio	Pr.Nr.4311Q-01892	1
fischar	Bicarbonato de sódio	6522101	6
Fischer/VDL	Bicarbonato de sódio	6521111	5
Gehe	Bicarbonato de sódio	11078315	1
Gehe	Bicarbonato de sódio	1203030-02	8
Gehe	Bicarbonato de sódio	12k09-N05	1
Caelo	Bicarbonato de sódio	13186711	1
Phönix	Bicarbonato de sódio	13186705	4
Phönix	Bicarbonato de sódio	13390515	1
Caelo	Bicarbonato de sódio	12324702	7
Caelo	Bicarbonato de sódio	12109205	6
Fagron	Bicarbonato de sódio	13B18-N03	6
5N Plus Lübeck Gmb…	Bismuto, subnitrato (pesado)	12146908	1
Caelo	Bismuto, subnitrato (pesado)	12146903	4
Caelo	Bismuto, subnitrato (pesado)	12146902	1
Caelo	Bismuto, subnitrato (pesado)	12146911	3
Caelo	Bismuto, subnitrato (pesado)	4513M-01186	1
Caelo	Bismuto, subnitrato (pesado)	12146913	2
Caelo	Bismuto, subnitrato (pesado)	M468105	1
Caelo	Bismuto, subnitrato (pesado)	10013208	1
Caelo	Bismuto, subnitrato (pesado)	10F09-N13	1
Caelo	Bismuto, subnitrato (pesado)	10013213	1
Caelo	Bismuto, subnitrato (pesado)	11052805	1
Caelo	Bismuto, subnitrato (pesado)	11052809	1
Caesar & Loretz/ Noweda	Bismuto, subnitrato (pesado)	12145701	1
Fagron	Bismuto, subnitrato (pesado)	1309211186	1
Fagron	Bismuto, subnitrato (pesado)	12C08-N06	3
Fagron	Bismuto, subnitrato (pesado)	12D26-N03	1
Fagron	Bismuto, subnitrato (pesado)	1001311186	1
Fagron	Bismuto, subnitrato (pesado)	13C15-N05	3
Fagron	Bismuto, subnitrato (pesado)	13H28-B04-291385	1
Fagron	Bismuto, subnitrato (pesado)	11D28-N16	1
Fagron	Bismuto, subnitrato (pesado)	13B25-N02	3
Fagron	Bismuto, subnitrato (pesado)	11/13-N01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Merck	Bismuto, subnitrato (pesado)	75419201	1
Noweda	Bismuto, subnitrato (pesado)	13/01-N02	1
Purren Apotheke	Bismuto, subnitrato (pesado)	11H31-N06	1
Sanacorp	Bismuto, subnitrato (pesado)	12146909	2
Caelo	Black cohosh (Cimicifuga ra…	10281112	1
Caelo	Black cohosh (Cimicifuga ra…	10281104	1
Caelo	Black cohosh (Cimicifuga ra…	10281118	2
Caelo	Black cohosh (Cimicifuga ra…	13142101	1
Caelo	Black cohosh (Cimicifuga ra…	13237907	1
Caelo	Black cohosh (Cimicifuga ra…	51981386	1
Caelo	Black cohosh (Cimicifuga ra…	13237903	1
Klenk	Black cohosh (Cimicifuga ra…	6721B141202	1
Caelo	Black cohosh (Cimicifuga ra…	13237901	2
Klenk	Black cohosh (Cimicifuga ra…	6721B130214	10
Klenk	Black cohosh (Cimicifuga ra…	B130528	2
Klenk	Black cohosh (Cimicifuga ra…	6721B1130528	1
Klenk	Black cohosh (Cimicifuga ra…	3794377	1
Klenk	Black cohosh (Cimicifuga ra…	6721B081208	1
Klenk	Black cohosh (Cimicifuga ra…	6721b130528	1
Kräuter Schulte	Black cohosh (Cimicifuga ra…	3308M-02176	1
Nachprüfung	Black cohosh (Cimicifuga ra…	10281113	1
Klenk	Black cohosh (Cimicifuga ra…	6721B130528	3
Caelo	Botão de algodão americano	12027506	1
Caelo	Botão de algodão americano	70864257	1
Klenk	Botão de algodão americano	3260A120828	1
Caelo	Botão de algodão americano	12027504	1
Fagron	Butirato de hidrocortisona	16j21-b01	1
Fagron	Butirato de hidrocortisona	15G08-B16-314883	1
Sigma-Aldrich	Butirato de sódio	Lot.091M-5302V	1

C

Supplier	Substance	Batch	Spectra
Akazie	Canela	20.09.2015	1
Akazien-Apo	Canela	Test	1
Caelo	Canela	11357909	1
Caelo	Canela	11357912	2
Caelo	Canela	12309902	3
Caelo	Canela	12309908	1
Caelo	Canela	25111307	1
Caelo	Canela	12309909	1
Caelo	Canela	13304401	2
Caelo	Canela	13304415	1
Caelo	Canela	13304402	2
Caelo	Canela	13304409	1
Caelo	Canela	13304407	1
Caelo	Canela	15151905	1
Caelo	Canela	16061702	1
Fargon / Gehe	Canela	15104201	1
Caelo	Canela	15151902	1
Caelo	Canela	16245105	1
Klenk	Canela	610A101018	1
Klenk	Canela	610A130927	1
siehe Protokoll	Canela	sieheProtokoll	1
Klenk	Canela do Ceilão, pulveriza…	614B160818	1
Klenk	Canela do Ceilão, pulveriza…	614B120411	2
Klenk	Canela do Ceilão, pulveriza…	611B100628	1
Klenk	Canela do Ceilão, pulveriza…	614B121010	2
Klenk	Canela do Ceilão, pulveriza…	614b121024	1
Klenk	Canela do Ceilão, pulveriza…	614a120411	1
Klenk	Canela do Ceilão, pulveriza…	615B130325	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Canela do Ceilão, pulveriza…	614B121024	4
AHD	Cânfora	17288306	18
Euro OTC	Cânfora	1210030-02	1
an	Cânfora	12344909	1
Caelo	Cânfora	13205502	1
Caelo	Cânfora	13195316	6
Caelo	Cânfora		1
Caelo	Cânfora	11286905	2
Caelo	Cânfora	3091203	1
Caelo	Cânfora	11032023	1
Caelo	Cânfora	11074509	1
Caelo	Cânfora	12054107	4
Caelo	Cânfora	120564113	1
Caelo	Cânfora	12054141	3
Caelo	Cânfora	12344905	2
Caelo	Cânfora	12054142	6
Caelo	Cânfora	11286910	1
Caelo	Cânfora	4101303	1
Caelo	Cânfora	12054114	2
Caelo	Cânfora	12243701	1
Caelo	Cânfora	13205512	2
Caelo	Cânfora	13205511	1
Caelo	Cânfora	13195311	1
Caelo	Cânfora	25041401	1
Caelo	Cânfora	13195314	5
Caelo	Cânfora	12061411	1
Caelo	Cânfora	13195316	1
Caelo	Cânfora	13205522	1
Caelo	Cânfora	13205522	3
Caelo	Cânfora	13195318	1
Caelo	Cânfora	13K28-04-294937	1
Caelo	Cânfora	13195322	7
Caelo	Cânfora	4031503	1
Caelo	Cânfora	13195327	1
Caelo	Cânfora	13195326	3
Caelo	Cânfora	14202807	3
Caelo	Cânfora	15097803	2
Caelo	Cânfora	15120901	2
Caelo	Cânfora	14310705	1
Caelo	Cânfora	15316807	7
Caelo	Cânfora	15320604	5
Caelo	Cânfora	1410710	1
Caelo	Cânfora	14310713	11
Caelo	Cânfora	15316819	7
Caelo	Cânfora	150622C	1
Caelo	Cânfora	140918C	1
Caelo	Cânfora	1531611	1
Caelo	Cânfora	15120902	1
Caelo	Cânfora	16209304	3
Caelo	Cânfora	14310710	2
Caelo	Cânfora	14310718	6
Caelo	Cânfora	15384201	1
Caelo	Cânfora	15397701	1
Caelo	Cânfora	16209305	11
Caelo	Cânfora	16235405	2
Caelo	Cânfora	14310722	3
Caelo	Cânfora	16235404	4
Caelo	Cânfora	16209306	1
Caelo	Cânfora	15/18.B11-321658	1
Caelo	Cânfora	162093029	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cânfora	17004304	1
Caelo	Cânfora	17004302	4
Caelo	Cânfora	17050605	30
Caelo	Cânfora	13111707	1
Caelo	Cânfora	13111708	1
Caelo	Cânfora	1531607	1
Caelo	Cânfora	17134703	4
Caelo	Cânfora	17288301	11
Caelo	Cânfora	17324104	10
Caelo	Cânfora	7061802	1
Caelo	Cânfora	7071801	1
Caelo	Cânfora	17288305	1
Caelo	Cânfora	18066404	9
Caelo	Cânfora	12091805	1
Caelo	Cânfora	12091808	1
Caelo	Cânfora	17325503	1
Caelo	Cânfora	17325502	1
Caelo	Cânfora	18019806	26
Caelo	Cânfora	6021901	1
Caelo	Cânfora	18019807	2
Caelo	Cânfora	18196902	1
Caelo	Cânfora	1728306	1
Caelo	Cânfora	17288360	1
Caelo	Cânfora	18196910	1
Caelo	Cânfora	18327910	2
Caelo	Cânfora	18196907	1
Caelo	Cânfora	192762009	2
Caelo	Cânfora	20003828001	1
Caelo	Cânfora	20004261002	1
Caelo	Cânfora	15086806	1
Caelo	Cânfora	16209301	12
Caelo	Cânfora	1536801	1
Caelo	Cânfora	13195301	1
Caelo	Cânfora	13195301	2
Caelo	Cânfora	13195304	1
Caelo	Cânfora	13195311	1
Caelo	Cânfora	16209309	24
Caelo	Cânfora	12054149	9
Caelo	Cânfora	444A170221	1
Caelo	Cânfora	13195318	1
Caelo	Cânfora	18327903P-191111-3	1
Caelo	Cânfora	18019803P-190506-3	1
Caelo	Cânfora	12228206	1
Caelo	Cânfora	62(17288306)	1
Caelo	Cânfora	3273	1
Caelo	Cânfora	14310706	1
Caelo	Cânfora	17050606	5
Caelo	Cânfora	12054151	2
Caelo	Cânfora	13195323	1
Caelo	Cânfora	15316805	1
Caelo	Cânfora	18108904	11
Caelo	Cânfora	14224304	1
Caelo	Cânfora	11286909	2
Caelo	Cânfora	2344905	1
Caelo	Cânfora	713A-01221	1
Caelo	Cânfora	914E-01221	1
Caelo	Cânfora	315E-01221	1
Caelo	Cânfora	5315I-01221	1
Caelo	Cânfora	218U-01221	1
Caelo	Cânfora	14310715	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cânfora	14224303	3
Caelo	Cânfora	1412023-01	7
Caelo	Cânfora	18198003	1
Caelo	Cânfora	18019603	1
Caelo	Cânfora	18327905	3
Caelo	Cânfora	18327909	2
Caelo	Cânfora	12228205	1
Caelo	Cânfora	12054124	2
Caelo	Cânfora	12054143	1
Caelo	Cânfora	2811Q-01221	1
Caelo	Cânfora	13205512	1
Caelo	Cânfora	15086801	1
Caelo	Cânfora	15316806	2
Caelo	Cânfora	15062701	1
Caelo	Cânfora	15316815	4
Caelo	Cânfora	16209310	1
Caelo	Cânfora	17004307	1
Caelo	Cânfora	13108106	2
Caelo	Cânfora	13205501	2
Caelo	Cânfora	19009704	5
Caelo	Cânfora	17004308	2
Caelo	Cânfora	14310705	14
Caelo	Cânfora	14310703	1
Caelo	Cânfora	13205511	2
Caelo	Cânfora	2803020-01	1
Caelo	Cânfora	14310709	6
Caelo	Cânfora	4444A150721	1
Caelo	Cânfora	13205517	1
Caelo	Cânfora	14310109	1
Caelo	Cânfora	15397704	5
Caelo	Cânfora	15316823	3
Caelo	Cânfora	17004301	21
Caelo	Cânfora	18019803	14
Caelo	Cânfora	12054105	1
Caelo	Cânfora	13195314	3
Caelo	Cânfora	13108118	2
Caelo	Cânfora	14G23-B04-301879	2
Caelo	Cânfora	15062702	3
Caelo	Cânfora	15316801	4
Caelo	Cânfora	15316812	1
Caelo	Cânfora	16235407	1
Caelo	Cânfora	16235402	1
Caelo	Cânfora	2015113782	1
Caelo	Cânfora	14310702	1
Caesar & Loretz GmbH	Cânfora	18019811	15
Caesar & Loretz GmbH	Cânfora	17288307	2
Caesar & Loretz GmbH	Cânfora	18327901	2
Caesar & Loretz GmbH	Cânfora	192762005	2
Caesar & Loretz Gm…	Cânfora	11032035	4
Caesar & Loretz Gm…	Cânfora	18019813	1
Caesar Loretz	Cânfora	18327903	13
Caesar&Loretz	Cânfora	14310719	1
Caesar/Noweda	Cânfora	1032	1
Caesar/Noweda	Cânfora	13195328	1
Calo/AHD	Cânfora	15086803	1
Camphor & Allied P…	Cânfora	16209302	1
Cealo/ Noweda	Cânfora	13108116	1
EuRho	Cânfora	2111E-01219	1
Euro OTC	Cânfora	1210030-02	4
Euro OTC	Cânfora	1202021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cânfora	113Q-01221	1
Euro OTC	Cânfora	121003001	1
Euro OTC	Cânfora	130313-02	1
Euro OTC	Cânfora	1309019-03	1
Euro OTC	Cânfora	1210030-01	7
Euro OTC	Cânfora	1101029-02/Ch241011	1
Euro OTC	Cânfora	1210030-01	1
Euro OTC	Cânfora	1406029-02	2
Euro OTC	Cânfora	121003002	1
Euro OTC	Cânfora	1202021-02	2
Euro OTC	Cânfora	1406029-01	3
Euro OTC	Cânfora	1101029-02	1
Euro OTC	Cânfora	1303013-02	11
euro/ Sanacorp	Cânfora	17050602	2
Euro OTC	Cânfora	821509	1
Euro OTC	Cânfora	1309019-02	1
Euro OTC	Cânfora	2803020-01	1
Euro OTC	Cânfora	1303013-01	5
Fagron	Cânfora	12G02-N09	1
Fagron	Cânfora	12D23-N03	1
Fagron	Cânfora	11K23-N04	1
Fagron	Cânfora	690442	1
Fagron	Cânfora	13H23-B40-291888	1
Fagron	Cânfora	13H23-B40-294116	1
Fagron	Cânfora	8082014A	1
Fagron	Cânfora	13h23-b40-294116	1
Fagron	Cânfora	14G23-B04-296868	1
Fagron	Cânfora	1309019-02	1
Fagron	Cânfora	13K28-B04-289340	1
Fagron	Cânfora	15/18-B11-321658	1
Fagron	Cânfora	17L01-B03	1
Fagron	Cânfora	13H23-B04-288376	1
Fagron	Cânfora	13K28-B04-294937	1
Fagron	Cânfora	14G23-B04-301878	3
Fagron	Cânfora	14G23-B04-299202	2
Fagron	Cânfora	27011	1
Fagron	Cânfora	825653	1
Fagron	Cânfora	14G23-B04	2
Fagron	Cânfora	13K28-B04	1
Fagron	Cânfora	13H23-B40-296252	1
Fagron	Cânfora	11H30-N15	1
Fagron	Cânfora	13K28-B04	2
Fagron	Cânfora	13K28_B04_294933	1
Fagron	Cânfora	15097801	1
Fagron	Cânfora	12B14-N09	1
Galke	Cânfora	23624	1
Gatt-Koller	Cânfora	1800202	3
Gehe	Cânfora	17134702	5
GEHE	Cânfora	16235408	5
Caelo	Cânfora	14224303	1
Caelo	Cânfora	17050605/1140418	1
Klenk	Cânfora	444A160817	8
Klenk	Cânfora	444A150721	1
Klenk	Cânfora	444A100826	1
Klenk	Cânfora	444A180815	3
Klenk	Cânfora	444A170224	4
Klenk	Cânfora	444A150721	1
Klenk	Cânfora	444A140526	5
L12	Cânfora	18108901	1
Caelo	Cânfora	15397705	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Nachprüfung	Cânfora	1616E-01221	1
Nachtestung-Verlän…	Cânfora	242/17	1
Noweda	Cânfora	1202021-01	3
Caelo	Cânfora	14202801	3
Phoenix	Cânfora	15316811	8
Phoenix	Cânfora	160209309	1
Phoenix	Cânfora	3382	1
Caelo	Cânfora	12054113	1
phönix	Cânfora	444a160817	1
Phönix Gotha	Cânfora	206/06	1
Caelo	Cânfora	2018-05-07-AISe	1
Post-Apotheke 22.0…	Cânfora	11032012	1
Sanacorp	Cânfora	444A130115	1
Sanacorp	Cânfora	14310720	2
Sanacorp	Cânfora	17004306	11
Sanacorp	Cânfora	18019802	9
Caelo	Cânfora	15097802	2
Caelo	Cânfora	18108902	1
Caelo	Cânfora	18108905	2
Vögele	Cânfora	2014101206	1
Vögele	Cânfora	2016114336	1
xxx	Cânfora	709E-01221	1
Caelo	Capim-limão, cortado	13149703	1
Caelo	Capim-limão, cortado	13341301	1
Caelo	Capim-limão, cortado	11301509	2
Caelo	Capim-limão, cortado	11301501	1
Klenk	Capim-limão, cortado	7721A130708	1
Klenk	Capim-limão, cortado	A120906	1
Klenk	Capim-limão, cortado	A130907	1
Klenk	Capim-limão, cortado	7721A120906	1
Caelo	Capim-limão, cortado	13149701	4
Caelo	Capim-limão, cortado	11301503	1
Wolf	Capim-limão, cortado	B654	1
apomix	Carbacol	12330703	1
Caelo	Carbonato de magnésio, pesado	2091303	1
Caelo	Carbonato de magnésio, pesado	13123505	1
Caelo	Carbonato de magnésio, pesado	13123502	1
Caelo	Carbonato de magnésio, pesado	7011404	1
Caelo	Carbonato de magnésio, pesado	13123504	2
Caelo	Carbonato de magnésio, pesado	12135404	1
Euro OTC	Carbonato de magnésio, pesado	1305024-01	1
Fagron	Carbonato de magnésio, pesado	12F20-N04	1
Euro OTC	Carbonato de magnésio, pesado	1211005-01	4
Caelo	Carbonato de sódio deca-hid…	11254706	1
Caelo	Carbonato de sódio deca-hid…	11254708	1
Caelo	Carbonato de sódio deca-hid…	12239810	2
Caelo	Carbonato de sódio deca-hid…	80136179	1
Caelo	Carbonato de sódio deca-hid…	13036907	1
Caelo	Carbonato de sódio deca-hid…	13036909	1
Caelo	Carbonato de sódio deca-hid…	13036910	1
Caelo	Carbonato de sódio deca-hid…	13036902	2
Caelo	Carbonato de sódio deca-hid…	12239806	1
Caelo	Carbonato de sódio deca-hid…	80136428	1
Phönix	Carbonato de sódio deca-hid…	13036904	2
Caelo	Cardo-mariano, planta	10365604	4
Caelo	Cardo-mariano, planta	10315909	1
Caelo	Cardo-mariano, planta	10315911	4
Caelo	Cardo-mariano, planta	10315907	1
Caelo	Cardo-mariano, planta	17121204	1
Caelo	Cardo-mariano, planta	10365601	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cardo-mariano, planta	1035911	1
Caelo	Cardo-mariano, planta	18041303	1
Caelo	Cardo-mariano, planta	intch:318080	1
Caelo	Cardo-mariano, planta	13130703	2
Caelo	Cardo-mariano, planta	1313702	1
Caelo	Cardo-mariano, planta	30101306	1
Caelo	Cardo-mariano, planta	13130701	2
Caelo	Cardo-mariano, planta	13130704	5
Caelo	Cardo-mariano, planta	10365605	1
Caelo	Cardo-mariano, planta	62607127	1
Caelo	Cardo-mariano, planta	13130701-3492411030	1
Caelo	Cardo-mariano, planta	13386703-3543411013	1
Caelo	Cardo-mariano, planta	13130702	3
Euro OTC	Cardo-mariano, planta	3701A-111207	1
Gehe	Cardo-mariano, planta	10365602	2
Klenk	Cardo-mariano, planta	3701B130318	5
Klenk	Cardo-mariano, planta	11041310	1
Klenk	Cardo-mariano, planta	3701B111117	1
Klenk	Cardo-mariano, planta	B110728	1
Klenk	Cardo-mariano, planta	3701a111207	1
Klenk	Cardo-mariano, planta	2011402	1
Klenk	Cardo-mariano, planta	3701A100916	2
Klenk	Cardo-mariano, planta	913E-01627	1
Klenk	Cardo-mariano, planta	3701A111207	11
Klenk	Cardo-mariano, planta	3701B120717	3
Caelo	Casca de cacau, cortada	19011303	1
Caelo	Casca de cacau, cortada	12126901	1
Caelo	Casca de cacau, cortada	12126907	1
Caelo	Casca de cacau, cortada	12126910	1
Caelo	Casca de cacau, cortada	12126905	2
Caelo	Casca de cacau, cortada	1216907	1
Caelo	Casca de canela	12148904	1
Klenk	Casca de canela	A101018	1
Klenk	Casca de canela	B121016	1
Klenk	Casca de canela	610A101018	1
Phönix	Casca de canela	610A130927	1
Sanacorp	Casca de canela	13231601	1
Caelo	Casca de canela pulverizada…	12242806	2
Caelo	Casca de canela pulverizada…	12242815	1
Caelo	Casca de canela pulverizada…	12242818	1
Klenk	Casca de canela pulverizada…	614B161128	1
Caelo	Casca de carvalho pulverizada	10261513	1
Caelo	Casca de cinchona, cortada	10381906	1
Caelo	Casca de cinchona, cortada	15301904	2
Caelo	Casca de cinchona, cortada	14009305	1
Klenk	Casca de cinchona, cortada	601B130415	1
Klenk	Casca de cinchona, cortada	601B130415	1
Bombastus	Casca de frângula	268407	1
Bombastus	Casca de frângula	270733	1
Bombastus	Casca de frângula	273926	1
Bombastus	Casca de frângula	275998	2
Bombastus	Casca de frângula	281284	2
Bombastus	Casca de frângula	278599	3
Bombastus	Casca de frângula	238812	1
Caelo	Casca de frângula	11254001	2
Caelo	Casca de frângula	11340801	1
Caelo	Casca de frângula	12185901	10
Caelo	Casca de frângula	10061301	1
Caelo	Casca de frângula	12186006	8
Caelo	Casca de frângula	13203008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Casca de frângula	6011402	1
Caelo	Casca de frângula	14163102	1
Caelo	Casca de frângula	eztetdt	1
Caelo	Casca de frângula	12186001	1
Caelo	Casca de frângula	12186003	1
Caelo	Casca de frângula	12186005	1
Caelo	Casca de frângula	1286003	1
Caelo	Casca de frângula	12186002	16
Caelo	Casca de frângula	121860006	1
Caesar&loretz,Phoenix	Casca de frângula	14163104	1
Finze	Casca de frângula	249091	1
Gehe	Casca de frângula	11254003	2
Gehe	Casca de frângula	11254004	4
Gehe	Casca de frângula	11254006	4
Klenk	Casca de frângula	661B110412	4
Klenk	Casca de frângula	6621B110412	1
Klenk	Casca de frângula	661B130306	1
Klenk	Casca de frângula	661B-090903	1
Klenk	Casca de frângula	661B-110412	1
Caelo	Casca de frângula	12186004	11
Caelo	Casca de hamamélis, cortada	12361301	1
Caelo	Casca de hamamélis, cortada	13123701	1
Caelo	Casca de hamamélis, cortada	13123703	1
Caelo	Casca de lapacho, cortada	19061301	1
Caelo	Casca de lapacho, cortada	13298308	1
Caelo	Casca de lapacho, cortada	11154506	1
Caelo	Casca de lapacho, cortada	2x11154506	1
Caelo	Casca de lapacho, cortada	12239303	2
Caelo	Casca de lapacho, cortada	12239305	8
Kenk / Phoenix	Casca de lapacho, cortada	5161A110204	1
Klenk	Casca de lapacho, cortada	13298302	1
Caelo	Casca de lapacho, cortada	13298305	1
Klenk	Casca de laranja, cortada	531A091125	3
Klenk	Casca de laranja, cortada	531A130204	5
Klenk	Casca de laranja, cortada	531a130204	1
Caelo	Casca de limão, cortada	12217402	1
Caelo	Casca de limão, cortada	12217401	1
Caelo	Casca de limão, cortada	12217404	1
Galke	Casca de limão, cortada	22975	1
Klenk	Casca de limão, cortada	621A130221	1
Klenk	Casca de limão, cortada	621A091016	1
Klenk	Casca de limão, cortada	B130521	1
Klenk	Casca de limão, cortada	A130221	3
Caelo	Casca de olmo, cortada	10347204	1
Caelo	Casca de olmo, cortada	12287902	2
Caelo	Casca de olmo, cortada	10347203	1
Klenk	Casca de olmo, cortada	841a120413	1
Klenk	Casca de olmo, cortada	841A1101120	1
Caelo	Casca de raiz de bérberis, ...	11083509	1
Caelo	Casca de raiz de bérberis, ...	55B110128	1
Caelo	Casca de raiz de bérberis, ...	12112606	5
Caelo	Casca de raiz de bérberis, ...	12112603	2
Caelo	Casca de raiz de bérberis, ...	12112605	1
Klenk	Casca de raiz de bérberis, ...	551B110128	4
Klenk	Casca de raiz de bérberis, ...	551B120320	1
Caelo	Casca de raiz de bérberis, ...	12112608	1
Bomba/AHD	Casca de salgueiro	280362	1
Bombastus	Casca de salgueiro	261615	1
Bombastus	Casca de salgueiro	277005	3
Bombastus	Casca de salgueiro	278458	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Casca de salgueiro	277847	1
Bombastus	Casca de salgueiro	288869	1
Bombastus	Casca de salgueiro	251385	1
Bombastus	Casca de salgueiro	292710	1
Bombastus	Casca de salgueiro	282270	1
Bombastus	Casca de salgueiro	281533	2
Bombastus	Casca de salgueiro	161594	1
Caelo	Casca de salgueiro	11073210	3
Caelo	Casca de salgueiro	11073201	1
Caelo	Casca de salgueiro	12185201	5
Caelo	Casca de salgueiro	21011302	1
Caelo	Casca de salgueiro	12185206	5
Caelo	Casca de salgueiro	11073208	1
Caelo	Casca de salgueiro	2185206	1
Caelo	Casca de salgueiro	12185208	12
Caelo	Casca de salgueiro	9071301	1
Caelo	Casca de salgueiro	13180702	4
Caelo	Casca de salgueiro	13180705	1
Caelo	Casca de salgueiro	12185204	4
Caelo	Casca de salgueiro	12185207	3
Caelo	Casca de salgueiro	13180701	1
Caelo	Casca de salgueiro	13180705-3530411072	1
Galke	Casca de salgueiro	20338	1
Klenk	Casca de salgueiro	811B100910	3
Klenk	Casca de salgueiro	B100910	6
Noweda	Casca de salgueiro	4609A-01305	1
Bombastus	Cascas de nozes	711B1206130	1
Caelo	Cascas de nozes	11016604	1
Caelo	Cascas de nozes	11325606	2
Caelo	Cascas de nozes	11325605	1
Caelo	Cascas de nozes	11016605	1
Caelo	Cascas de nozes	11325603	1
Fiebig 16.11.12 ek:2,35	Cascas de nozes	711B111020	5
Gehe	Cascas de nozes	711B110128	3
Klenk	Cascas de nozes	711B120613	3
Klenk	Cascas de nozes	711B080806	1
Klenk	Cascas de nozes	711b120613	1
Klenk	Cascas de nozes	711B120906	2
Anzag ek:2,50EUR 15.09.12	Castanha-da-índia (Aesculus…	2551B111013	7
Apotheke Bühlau	Castanha-da-índia (Aesculus…	100416	1
Caelo	Castanha-da-índia (Aesculus…	11063503	2
Gehe	Castanha-da-índia (Aesculus…	2551B131024	1
Klenk	Castanha-da-índia (Aesculus…	255100903	1
Klenk	Castanha-da-índia (Aesculus…	N130124	2
Klenk	Castanha-da-índia (Aesculus…	2551N130124	3
Klenk	Castanha-da-índia (Aesculus…	2551B081223	1
Caelo	Caule de doce-amarga (Solan…	10375605	2
Caelo	Caule de doce-amarga (Solan…	10375607	1
Caelo	Caule de doce-amarga (Solan…	132564301	1
Caelo	Caule de doce-amarga (Solan…	13254301	1
Caelo	Caule de doce-amarga (Solan…	103745604	1
Klenk	Caule de doce-amarga (Solan…	5601A080513	3
Caelo	Caule de ginja, cortado	10367019	1
Caelo	Caule de ginja, cortado	12042301	1
Caelo	Caule de ginja, cortado	10367014	1
Caelo	Caule de ginja, cortado	12042307	1
Caelo	Caulim, pesado	11041610	1
Caelo	Caulim, pesado	11350106	2
Caelo	Caulim, pesado	11350115	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Caulim, pesado	10176518	1
Caelo	Caulim, pesado	11350124	4
Caelo	Caulim, pesado	11350107	1
Caelo	Caulim, pesado	82043269	1
Caelo	Caulim, pesado	13041803	1
Caelo	Caulim, pesado	13041835	2
Caelo	Caulim, pesado	13041801	2
Caelo	Caulim, pesado	13041834	1
Caelo	Caulim, pesado	11350107	5
Caelo	Caulim, pesado	13041803	1
Caelo	Caulim, pesado	11350125	4
Caelo	Caulim, pesado	13041835	1
Caelo	Caulim, pesado	63033516	1
Klenk	Caulim, pesado	424A100819	2
Klenk	Caulim, pesado	45131I01190	1
Klenk	Caulim, pesado	424A130507	4
Klenk	Caulim, pesado	424A130507	2
Aurica / 11	Cavalinha (Equisetum arvens…	521302898	1
Bomba/AHD	Cavalinha (Equisetum arvens…	280449	3
Bombastus	Cavalinha (Equisetum arvens…	273963	1
Bombastus	Cavalinha (Equisetum arvens…	275891	3
Bombastus	Cavalinha (Equisetum arvens…	264100	1
Bombastus	Cavalinha (Equisetum arvens…	272552	2
Bombastus	Cavalinha (Equisetum arvens…	265924	1
Bombastus	Cavalinha (Equisetum arvens…	278107	1
Bombastus	Cavalinha (Equisetum arvens…	18111304	1
Bombastus	Cavalinha (Equisetum arvens…	6011401	1
Bombastus	Cavalinha (Equisetum arvens…	280647	1
Bombastus	Cavalinha (Equisetum arvens…	268321	1
Bombastus	Cavalinha (Equisetum arvens…	264101	1
Bombastus	Cavalinha (Equisetum arvens…	274714	1
Caelo	Cavalinha (Equisetum arvens…	13344309	3
Caelo	Cavalinha (Equisetum arvens…	11021901	1
Caelo	Cavalinha (Equisetum arvens…	11076302	2
Caelo	Cavalinha (Equisetum arvens…	3091201	1
Caelo	Cavalinha (Equisetum arvens…	11076306	6
Caelo	Cavalinha (Equisetum arvens…	8101201	1
Caelo	Cavalinha (Equisetum arvens…	17101203	1
Caelo	Cavalinha (Equisetum arvens…	20111212	1
Caelo	Cavalinha (Equisetum arvens…	11076303	13
Caelo	Cavalinha (Equisetum arvens…	2658181	1
Caelo	Cavalinha (Equisetum arvens…	10328901	1
Caelo	Cavalinha (Equisetum arvens…	1288804	1
Caelo	Cavalinha (Equisetum arvens…	8041301	1
Caelo	Cavalinha (Equisetum arvens…	8051302	1
Caelo	Cavalinha (Equisetum arvens…	12288802	2
Caelo	Cavalinha (Equisetum arvens…	6081304	1
Caelo	Cavalinha (Equisetum arvens…	311042	1
Caelo	Cavalinha (Equisetum arvens…	13159702	10
Caelo	Cavalinha (Equisetum arvens…	13159706	5
Caelo	Cavalinha (Equisetum arvens…	13091301	1
Caelo	Cavalinha (Equisetum arvens…	13159704	6
Caelo	Cavalinha (Equisetum arvens…	9101313	1
Caelo	Cavalinha (Equisetum arvens…	30101305	1
Caelo	Cavalinha (Equisetum arvens…	13344305	1
Caelo	Cavalinha (Equisetum arvens…	2011408	1
Caelo	Cavalinha (Equisetum arvens…	13344304	5
Caelo	Cavalinha (Equisetum arvens…	13344311	1
Caelo	Cavalinha (Equisetum arvens…	13350301	1
Caelo	Cavalinha (Equisetum arvens…	13350309	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cavalinha (Equisetum arvens…	15015404	1
Caelo	Cavalinha (Equisetum arvens…	10328915	1
Caelo	Cavalinha (Equisetum arvens…	11021904	1
Caelo	Cavalinha (Equisetum arvens…	11076307	1
Caelo	Cavalinha (Equisetum arvens…	12288808	9
Caelo	Cavalinha (Equisetum arvens…	282573	1
Caelo	Cavalinha (Equisetum arvens…	13200201	1
Caelo	Cavalinha (Equisetum arvens…	10375520	1
Caelo	Cavalinha (Equisetum arvens…	13159705-3387310190	1
Caelo	Cavalinha (Equisetum arvens…	13153702	1
Caelo	Cavalinha (Equisetum arvens…	1359702	1
Caelo	Cavalinha (Equisetum arvens…	13159705	6
Caelo	Cavalinha (Equisetum arvens…	13344303	6
Caelo	Cavalinha (Equisetum arvens…	12288809	3
Caelo	Cavalinha (Equisetum arvens…	13159702-3464312101	1
Caelo	Cavalinha (Equisetum arvens…	13344302	3
Caesar & Loretz Gm…	Cavalinha (Equisetum arvens…	10375510	2
Caesar & Loretz Gm…	Cavalinha (Equisetum arvens…	12288801	16
Euro OTC	Cavalinha (Equisetum arvens…	3831A130610	5
Finze	Cavalinha (Equisetum arvens…	11076305	8
Galke	Cavalinha (Equisetum arvens…	19663	5
Galke	Cavalinha (Equisetum arvens…	22061	1
Gehe	Cavalinha (Equisetum arvens…	10375515	1
Gehe	Cavalinha (Equisetum arvens…	11076301	4
Gehe	Cavalinha (Equisetum arvens…	12288803	14
Klenk	Cavalinha (Equisetum arvens…	3831A111124	4
Hepart AG	Cavalinha (Equisetum arvens…	B-695,kbA	1
Hubertus Apotheke	Cavalinha (Equisetum arvens…	3831C140403	1
KBA Ware	Cavalinha (Equisetum arvens…	21879	6
Klenk	Cavalinha (Equisetum arvens…	3831a120611	1
Klenk	Cavalinha (Equisetum arvens…	2213U01642	1
Klenk	Cavalinha (Equisetum arvens…	3831A121018	6
Klenk	Cavalinha (Equisetum arvens…	3831A120903	8
Klenk	Cavalinha (Equisetum arvens…	3831A110922	1
Klenk	Cavalinha (Equisetum arvens…	3831A120018	1
Klenk	Cavalinha (Equisetum arvens…	3831A1230726	1
Klenk	Cavalinha (Equisetum arvens…	3831c131104	1
Klenk	Cavalinha (Equisetum arvens…	3831C131104	1
Klenk	Cavalinha (Equisetum arvens…	3831A11124	1
Klenk	Cavalinha (Equisetum arvens…	4713U01642	1
Klenk	Cavalinha (Equisetum arvens…	3831A110601	1
Klenk	Cavalinha (Equisetum arvens…	3831A120529	8
Klenk	Cavalinha (Equisetum arvens…	4413Q1642	1
Klenk	Cavalinha (Equisetum arvens…	3831A120611	10
Noweda	Cavalinha (Equisetum arvens…	12231401	6
Klenk	Cavalinha (Equisetum arvens…	3831A120726	18
Caelo	Cavalinha (Equisetum arvens…	13344306	1
Caelo	Cavalinha (Equisetum arvens…	12288804	11
Phönix	Cavalinha (Equisetum arvens…	12288807	2
Sanacorp	Cavalinha (Equisetum arvens…	13344307	1
Caelo	Cavalinha (Equisetum arvens…	10375507	2
Caelo	Cavalinha (Equisetum arvens…		2
Wolf	Cavalinha (Equisetum arvens…	B-695	1
Wolf	Cavalinha (Equisetum arvens…	B233885	4
-	Celidônia maior	810I-01632	1
Klenk	Celidônia maior	1406111632	1
Caelo	Celidônia maior	311092	1
Galke	Celidônia maior	20937	3
Klenk	Celidônia maior	3731A110301	6
Klenk	Celidônia maior	3731A120611	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Celidônia maior	4711E-01632	1
Klenk	Celidônia maior	3731A130904	5
Klenk	Celidônia maior	3731B100205	1
Klenk	Celidônia maior	3731K120904	4
Bombastus	Centaurea (Centaurium erythraea)	277598	3
Aurica/Phönix	Centaurea (Centaurium erythraea)	520702152	1
Caelo	Centaurea (Centaurium erythraea)	12268608	10
Caelo	Centaurea (Centaurium erythraea)	11097605	2
Caelo	Centaurea (Centaurium erythraea)	11097609	3
Caelo	Centaurea (Centaurium erythraea)	10104012	1
Caelo	Centaurea (Centaurium erythraea)	8021302	1
Caelo	Centaurea (Centaurium erythraea)	15224102	1
Caelo	Centaurea (Centaurium erythraea)	12268606	14
Caelo	Centaurea (Centaurium erythraea)	12379601	1
Caelo	Centaurea (Centaurium erythraea)	11097602	1
Caelo	Centaurea (Centaurium erythraea)	3711B120628	1
Caelo	Centaurea (Centaurium erythraea)	12268601	3
Caelo	Centaurea (Centaurium erythraea)	12268605	4
Caelo	Centaurea (Centaurium erythraea)	12268602	19
Caelo	Centaurea (Centaurium erythraea)	16240512	1
Caelo	Centaurea (Centaurium erythraea)	18029609	1
Finze	Centaurea (Centaurium erythraea)	11097610	1
Galke	Centaurea (Centaurium erythraea)	9721	1
Klenk	Centaurea (Centaurium erythraea)	3711B111216	1
Klenk	Centaurea (Centaurium erythraea)	B120628	1
Klenk	Centaurea (Centaurium erythraea)	3711B-111216	1
Phoenix	Centaurea (Centaurium erythraea)	11097612	9
Phönix	Centaurea (Centaurium erythraea)	11093612	2
Caelo	Chá de Java (Orthosiphon st…	20111207	1
Caelo	Chá de Java (Orthosiphon st…	31121203	1
Caelo	Chá de Java (Orthosiphon st…	2221B121112	16
Caelo	Chá de Java (Orthosiphon st…	12225702	1
Caelo	Chá de Java (Orthosiphon st…	21061304	1
Caelo	Chá de Java (Orthosiphon st…	28101305	1
Caelo	Chá de Java (Orthosiphon st…	12225704	3
Caelo	Chá de Java (Orthosiphon st…	13258804	3
Caelo	Chá de Java (Orthosiphon st…	2221A110825	2
Caelo	Chá de Java (Orthosiphon st…	11212901	1
Klenk	Chá de Java (Orthosiphon st…	2221B12112	1
Klenk	Chá de Java (Orthosiphon st…	2221B110718	6
Klenk	Chá de Java (Orthosiphon st…	B110718	1
Klenk	Chá de Java (Orthosiphon st…	B121112	3
Klenk	Chá de Java (Orthosiphon st…	17121304	1
Caelo	Chá de Java (Orthosiphon st…	13258802	2
VDL	Chá de Java (Orthosiphon st…	2221B101213	1
Kräuter Schulte	Chá vermelho	52029	1
-	Chicória, planta (Cichorium…	4411I-01634	1
Caelo	Chicória, planta (Cichorium…	12034302	1
Caelo	Chicória, planta (Cichorium…	12034303	3
Caelo	Chicória, planta (Cichorium…	12354302	3
Caelo	Chicória, planta (Cichorium…	14031315	1
Caelo	Chicória, planta (Cichorium…	12354304	1
Caelo	Chicória, planta (Cichorium…	12354306	1
Caelo	Chicória, planta (Cichorium…	12369102	3
Caelo	Chicória, planta (Cichorium…	12034301	2
Klenk	Chicória, planta (Cichorium…	3751A120123	2
Klenk	Chicória, planta (Cichorium…	A120123	2
Klenk	Chicória, planta (Cichorium…	3751A080902	1
Klenk	Chicória, planta (Cichorium…	3751A120307	7
Klenk	Chicória, planta (Cichorium…	3751a120307	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Chicória, planta (Cichorium…	3751c120614	1
Klenk	Chicória, planta (Cichorium…	3751A-100118	1
Klenk	Chicória, planta (Cichorium…	4510I-01634	1
Sanacorp	Chicória, planta (Cichorium…	12369101	6
Klenk	Chicória, raiz (Cichorium i…	66221A101202	1
Caelo	Chicória, raiz (Cichorium i…	6221A101202	4
Caelo	Chicória, raiz (Cichorium i…	11374501	1
Caelo	Chicória, raiz (Cichorium i…	11374504	3
Caelo	Chicória, raiz (Cichorium i…	11374506	1
Caelo	Chicória, raiz (Cichorium i…	6221As101202	1
Caelo	Chicória, raiz (Cichorium i…	11081803	1
Caelo	Chicória, raiz (Cichorium i…	11374510	2
Caelo	Chicória, raiz (Cichorium i…	91338319	1
Klenk	Chicória, raiz (Cichorium i…	6221A090311	1
Klenk	Chicória, raiz (Cichorium i…	6221N130201	1
Klenk	Chicória, raiz (Cichorium i…	A130304	1
Klenk	Chicória, raiz (Cichorium i…	6221A130304	1
Kräuter Schulte	China Pai Mu Tan	52783	1
Fagron	Cinarizina	13H01-N07	4
Fagron	Cinarizina	14D09-B01-292883	1
Fagron	Cinarizina	14D09-B01	3
Fagron	Cinarizina	8D11-N04	1
Fagron	Cinarizina	13I26-N22	1
Fagron	Cinarizina	13I26-N22	1
Fagron	Clobetasol-17-propionato 1:…	12A03-N03	1
Fagron	Clobetasol-17-propionato 1:…	11k04-n17	1
Fagron	Clobetasol-17-propionato 1:…	12|19-N01	1
Fagron	Clobetasol-17-propionato 1:…	12l19-N01	1
Fagron	Clobetasol-17-propionato 1:…	12I19-N01	2
Fagron	Clobetasol-17-propionato 1:…	12K08-N02	2
Fagron	Clobetasol-17-propionato 1:…	13W16-N01	1
Fagron	Clobetasol-17-propionato 1:…	12L19-N06	1
Fagron	Clobetasol-17-propionato 1:…	12/19-No1	1
Fagron	Clobetasol-17-propionato 1:…	12/19-N01003637	1
Caelo	Cloreto de amônio	10176319	2
Caelo	Cloreto de amônio	12240302	4
Caelo	Cloreto de amônio	12356101	3
Caelo	Cloreto de amônio	10176309	1
Euro OTC	Cloreto de amônio	1212017-01	2
Euro OTC	Cloreto de amônio	1303029-01	1
Euro OTC	Cloreto de amônio	1203029-01	1
Euro OTC	Cloreto de amônio	512A-01104	1
Caelo	Cloreto de cálcio di-hidratado	12341409	1
Caelo	Cloreto de cálcio di-hidratado	11230921	2
Caelo	Cloreto de cálcio di-hidratado	12341404	2
Caelo	Cloreto de cálcio di-hidratado	11230915	1
Caelo	Cloreto de cálcio di-hidratado	12341406	1
Caelo	Cloreto de cálcio di-hidratado	12B09-N11	1
EUro/AHD	Cloreto de cálcio di-hidratado	1205014-02	2
Caelo	Cloreto de cálcio di-hidratado	8237314	1
Caelo	Cloreto de metilrosanilínio	9238107	1
Caelo	Cloreto de metilrosanilínio	12H28-N06	1
Caelo	Cloreto de metilrosanilínio	3455360	1
Caelo	Cloreto de metilrosanilínio	13184801	1
Caelo	Cloreto de metilrosanilínio	12H28-No6	1
Caelo	Cloreto de metilrosanilínio	9238109	1
Caelo	Cloreto de metilrosanilínio	9238106	1
Fagron	Cloreto de metilrosanilínio	12H28_N06	1
Fagron	Cloreto de metilrosanilínio	13H28-N03	2
Fagron	Cloreto de metilrosanilínio	1989	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cloreto de metilrosanilínio	13G03N11	1
Fagron	Cloreto de metilrosanilínio	13H28-No3	1
Fagron	Cloreto de metilrosanilínio	13G03-N011	1
Fagron	Cloreto de metilrosanilínio	13G03-N11	1
Fagron	Cloreto de metilrosanilínio	13H28-N03	18
Fagron	Cloreto de metilrosanilínio	13H28-N03-0161-1030	1
Fagron	Cloreto de metilrosanilínio	12-17-N050109-140	1
Fagron	Cloreto de metilrosanilínio	12D19-N01	1
Fagron	Cloreto de metilrosanilínio	13H28-NO3	1
Fagron	Cloreto de metilrosanilínio	13G03-N11	1
Fagron	Cloreto de metilrosanilínio	12I17-N05	1
Noweda	Cloreto de metilrosanilínio	9238104	1
Noweda	Cloreto de metilrosanilínio	12H28-N06	1
Noweda	Cloreto de metilrosanilínio	2159	2
Caelo	Cloreto de metilrosanilínio	12/17-N05	1
phönix	Cloreto de metilrosanilínio	13184811	1
Fagron	Cloridrato de (R,S)-epinefrina	14A22-B05	1
Fagron	Cloridrato de (R,S)-epinefrina	2021503	1
Fagron	Cloridrato de (R,S)-epinefrina	10022015E	1
Fagron	Cloridrato de (R,S)-epinefrina	14a22-B05	1
Fagron	Cloridrato de (R,S)-epinefrina	16H23-B98-325052	1
Euro OTC	Cloridrato de betaína	1202008-01	1
Euro OTC	Cloridrato de betaína	L1701040-01	1
Euro OTC	Cloridrato de betaína	1305027-01	2
Euro OTC	Cloridrato de betaína	L1510011-03	1
Euro OTC	Cloridrato de betaína	1510011-02	1
Euro OTC	Cloridrato de betaína	L1412019-01	1
Fagron	Cloridrato de betaína	12C20-N09	1
Fagron	Cloridrato de betaína	24091301	1
Fagron	Cloridrato de betaína	15121401	1
Gatt-Koller	Cloridrato de betaína	2970/07102910	1
Fagron	Cloridrato de betaína	13G29-B02-294870	1
Fagron	Cloridrato de cinchocaína	12F25-N10	1
Phönix	Cloridrato de cinchocaína	13E13-N07	1
Fagron	Cloridrato de drofenina	12D04-N03	1
Fagron	Cloridrato de drofenina	11J24-N01	1
Caelo	Cloridrato de oxicodona	17270202	2
Caelo	Cloridrato de oxicodona	12268912	1
Caelo	Cloridrato de oxicodona	15220205	1
Caelo	Cloridrato de prometazina	11352305	1
Caelo	Cloridrato de prometazina	19051805	1
Caelo	Cloridrato de prometazina	17058601	2
Caelo	Cloridrato de prometazina	13119211	1
Bombastus	Coentro	263733	1
Bombastus	Coentro	306310	1
Caelo	Coentro	13010304	1
Caelo	Coentro	12080901	2
Caelo	Coentro	14031316	1
Caelo	Coentro	13010302	2
Caelo	Coentro	27061305	1
Caelo	Coentro	4091305	1
Caelo	Coentro	13010306	2
Caelo	Coentro	16010209	1
Caelo	Coentro	12080906	1
Caelo	Coentro	9285707	1
Caelo	Coentro	16010201	1
Caesar/Noweda	Coentro	2010M-01539	1
Klenk	Coentro	2790A161111	5
Caelo	Coentro	12080905	1
Klenk	Coentro	2790A121023	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Coentro	A121023	3
Klenk	Coentro	2790A130129	2
Klenk	Coentro	2709A130129	1
Klenk	Coentro	2790A151117	1
Klenk	Coentro	2790a121023	1
Caelo	Coentro	18010209	1
sanacorp;3,32;18.06.15	Coentro	13299495	1
Fagron	Colofônia	15186807	8
Euro OTC	Concentrado seco de colecal…	1012025-01	1
Euro OTC	Concentrado seco de colecal…	1602019-02	5
Euro OTC	Concentrado seco de colecal…	1608002-01	15
Euro OTC	Concentrado seco de colecal…	1508032-01	2
Euro OTC	Concentrado seco de colecal…	1701053-01	11
Euro OTC	Concentrado seco de colecal…	150803201	1
Euro OTC	Concentrado seco de colecal…	1707027-01	17
Euro OTC	Concentrado seco de colecal…	1801038-01	4
Euro OTC	Concentrado seco de colecal…	1802014-01	17
Euro OTC	Concentrado seco de colecal…	170153-01	5
Euro OTC	Concentrado seco de colecal…	1806003-01	28
Euro OTC	Concentrado seco de colecal…	2001007-01	1
Euro OTC	Concentrado seco de colecal…	1502021-01	1
Euro OTC	Concentrado seco de colecal…	1901050-01	4
Euro OTC	Concentrado seco de colecal…	1906009-01	8
Euro OTC	Concentrado seco de colecal…	1906009-02	5
Euro OTC	Concentrado seco de colecal…	1210051-01	1
Euro OTC	Concentrado seco de colecal…	1602019-01	2
Euro OTC	Concentrado seco de colecal…	L1403012-01	1
Euro OTC	Concentrado seco de colecal…	1806003-02	1
Bombastus	Confrei, cortado	281531	1
Klenk	Confrei, cortado	4561B100518	2
Caelo	Contas secas Caelo laranja	11005811	1
Caelo	Cravo	5398872	1
Caelo	Cravo	12095802	1
Caelo	Cravo	11233305	1
Caelo	Cravo	12095807	5
Caelo	Cravo	12095806	2
Caelo	Cravo	12266505	1
Caelo	Cravo	13371309	1
Caelo	Cravo	16207802	1
Caelo	Cravo	14057602	1
Klenk	Cravo	1260A110608	5
Klenk	Cravo	1260A100617	2
Klenk	Cravo	1260A101223	1
Klenk	Cravo	A120328	1
Klenk	Cravo	1260A120328	6
Klenk	Cravo	1260A130903	3
Klenk	Cravo	1260A150304	2
Caelo	Cravo pulverizado (especiaria)	14180001	1
Caelo	Cravo pulverizado (especiaria)	12355303	1
Creapure	Creatina	515941	1
Degussa / falcento	Creatina	422031	1
Phönix	Creatina	mysjhskeu	1
Caelo	Cubeba (Piper cubeba)	11081903	1
Caelo	Cumaru (Dipteryx odorata)	1078C	1
Caelo	Cumaru (Dipteryx odorata)	12145101	2
Caelo	Cumaru (Dipteryx odorata)	12144101	1
Caelo	Cumaru (Dipteryx odorata)	20111312	1
Noweda	Cumaru (Dipteryx odorata)	1040A111026	1
Caelo	Cúrcuma, rizoma	12136504	1
Caelo	Cúrcuma, rizoma	12136506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cúrcuma, rizoma	12136507	1
Caelo	Cúrcuma, rizoma	1213650	1
Caelo	Cúrcuma, rizoma	13360204	2
Caelo	Cúrcuma, rizoma	15158001	2
Caelo	Cúrcuma, rizoma	15158001	2
Caelo	Cúrcuma, rizoma	15372603	1
Caelo	Cúrcuma, rizoma	16344604	2
Caelo	Cúrcuma, rizoma	15207601	1
Caelo	Cúrcuma, rizoma	12136501	2
Caelo	Cúrcuma, rizoma	12136503	2
Galke	Cúrcuma, rizoma	20184	1
Galke	Cúrcuma, rizoma	23123	1
Klenk	Cúrcuma, rizoma	6741B121030	1

D

Supplier	Substance	Batch	Spectra
Falcento	D-(+)-manose	R-4638	1
Falcento	D-(+)-manose	R-4639	1
Falcento	D-(+)-manose	R4640	1
Falcento	D-(+)-manose	R-4641	1
Giusto Faravelli	D-(+)-manose	161004/1710215001	1
Caelo	Dapsona	18279201	4
Caelo	Dapsona	17031101	2
Caelo	Dapsona	19113501	3
Caesar & Loretz GmbH	Dapsona	191135001	1
Caelo	Dente-de-leão (Taraxacum of…	12363104	3
Caelo	Dente-de-leão (Taraxacum of…	10024710	1
Caelo	Dente-de-leão (Taraxacum of…	11003307	1
Caelo	Dente-de-leão (Taraxacum of…	11003311	2
Caelo	Dente-de-leão (Taraxacum of…	12363102	2
Caelo	Dente-de-leão (Taraxacum of…	12363103	1
Caelo	Dente-de-leão (Taraxacum of…	12363107	1
Caelo	Dente-de-leão (Taraxacum of…	12367916	1
Caelo	Dente-de-leão (Taraxacum of…	12363109	2
Caelo	Dente-de-leão (Taraxacum of…	12363108	2
Caelo	Dente-de-leão (Taraxacum of…	12363110	1
Caelo	Dente-de-leão (Taraxacum of…	13329705	1
Caelo	Dente-de-leão (Taraxacum of…	13329708	1
Caelo	Dente-de-leão (Taraxacum of…	14166502	1
Caelo	Dente-de-leão (Taraxacum of…	15096601	1
Caelo	Dente-de-leão (Taraxacum of…	15407703	1
Caelo	Dente-de-leão (Taraxacum of…	16161308	1
Caelo	Dente-de-leão (Taraxacum of…	15407703	1
Caelo	Dente-de-leão (Taraxacum of…	13329702	10
Caelo	Dente-de-leão (Taraxacum of…	16161303	1
Caelo	Dente-de-leão (Taraxacum of…	14166504	1
Caelo	Dente-de-leão (Taraxacum of…	14376602	1
Caelo	Dente-de-leão (Taraxacum of…	12363106	1
Caelo	Dente-de-leão (Taraxacum of…	11003313	1
Caelo	Dente-de-leão (Taraxacum of…	14166501	1
Caelo	Dente-de-leão (Taraxacum of…	14376603	1
Galke	Dente-de-leão (Taraxacum of…	126302	1
Galke	Dente-de-leão (Taraxacum of…	20658	1
Caelo	Dente-de-leão (Taraxacum of…	1140317	1
Klenk	Dente-de-leão (Taraxacum of…	6621A120208	6
Klenk	Dente-de-leão (Taraxacum of…	6621A110420	1
Klenk	Dente-de-leão (Taraxacum of…	6101202	1
Klenk	Dente-de-leão (Taraxacum of…	A120606	1
Klenk	Dente-de-leão (Taraxacum of…	N130813	1
Klenk	Dente-de-leão (Taraxacum of…	6621A160111	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier		Substance	Batch	Spectra
Klenk		Dente-de-leão (Taraxacum of…	6621B170112	1
Klenk		Dente-de-leão (Taraxacum of…	6621N130813	6
Klenk		Dente-de-leão (Taraxacum of…	6621A140114	3
Klenk		Dente-de-leão (Taraxacum of…	6621A140114	3
Klenk		Dente-de-leão (Taraxacum of…	6621A120606	15
Klenk		Dente-de-leão (Taraxacum of…	6621A141027	5
noweda		Dente-de-leão (Taraxacum of…		1
Anzag		Dente-de-Leão, planta com raiz	274030	1
Anzag ek:3,16EUR	10.05.13	Dente-de-Leão, planta com raiz	6611B130321	1
Anzag ek:3.16EUR	25.10.12	Dente-de-Leão, planta com raiz	6611B110131	1
Aurica		Dente-de-Leão, planta com raiz	521200197	1
Bombastus		Dente-de-Leão, planta com raiz	258809	1
Bombastus		Dente-de-Leão, planta com raiz	271272	5
Bombastus		Dente-de-Leão, planta com raiz	274030	5
Bombastus		Dente-de-Leão, planta com raiz	280363	5
Bombastus		Dente-de-Leão, planta com raiz	285264	1
Bombastus		Dente-de-Leão, planta com raiz	290125	1
Bombastus		Dente-de-Leão, planta com raiz	275126	1
Bombastus		Dente-de-Leão, planta com raiz	280363-3385310110	1
Bombastus		Dente-de-Leão, planta com raiz	282916	7
Caelo		Dente-de-Leão, planta com raiz	20111202	1
Caelo		Dente-de-Leão, planta com raiz	13108801	4
Caelo		Dente-de-Leão, planta com raiz	11030309	2
Caelo		Dente-de-Leão, planta com raiz	806212165	1
Caelo		Dente-de-Leão, planta com raiz	8111205	1
Caelo		Dente-de-Leão, planta com raiz	12236003	3
Caelo		Dente-de-Leão, planta com raiz	12236002	8
Caelo		Dente-de-Leão, planta com raiz	2112122165	1
Caelo		Dente-de-Leão, planta com raiz	11371903	1
Caelo		Dente-de-Leão, planta com raiz	11030305	1
Caelo		Dente-de-Leão, planta com raiz	13019802	19
Caelo		Dente-de-Leão, planta com raiz	13018902	1
Caelo		Dente-de-Leão, planta com raiz	Int.Ch:318090	1
Caelo		Dente-de-Leão, planta com raiz	13199202	2
Caelo		Dente-de-Leão, planta com raiz	17121305	1
Caelo		Dente-de-Leão, planta com raiz	13317903	1
Caelo		Dente-de-Leão, planta com raiz	Ch.-B.:13019802	1
Caelo		Dente-de-Leão, planta com raiz	11030313	2
Caelo		Dente-de-Leão, planta com raiz	12236001	3
Caelo		Dente-de-Leão, planta com raiz	6611B100902	1
Caelo		Dente-de-Leão, planta com raiz	18035117	1
Caelo		Dente-de-Leão, planta com raiz	19114404	1
Caelo		Dente-de-Leão, planta com raiz	19114406	1
Caelo		Dente-de-Leão, planta com raiz	13019805	1
Caelo		Dente-de-Leão, planta com raiz	13019802-3395310101	1
Caelo		Dente-de-Leão, planta com raiz	12236005	5
Caelo		Dente-de-Leão, planta com raiz	1103011	1
Caelo		Dente-de-Leão, planta com raiz	13019801	5
Caelo		Dente-de-Leão, planta com raiz	11030311	2
Caelo		Dente-de-Leão, planta com raiz	11030314	4
Caelo		Dente-de-Leão, planta com raiz	13108802	11
Caelo		Dente-de-Leão, planta com raiz	18046901	1
Caelo		Dente-de-Leão, planta com raiz	7341703	1
Caelo		Dente-de-Leão, planta com raiz	18035103	1
Caelo		Dente-de-Leão, planta com raiz	18035108	3
Caelo		Dente-de-Leão, planta com raiz	18035113	1
Euro OTC		Dente-de-Leão, planta com raiz	11030312	4
Galke		Dente-de-Leão, planta com raiz	20531	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Galke	Dente-de-Leão, planta com raiz	22093	2
Gehe	Dente-de-Leão, planta com raiz	6611B110104	1
Gehe	Dente-de-Leão, planta com raiz	13019803	1
Hedinger	Dente-de-Leão, planta com raiz	10121614	1
Klenk	Dente-de-Leão, planta com raiz	6611B110131	1
Klenk	Dente-de-Leão, planta com raiz	6611B160613	1
Klenk	Dente-de-Leão, planta com raiz	6611B120620	19
Klenk	Dente-de-Leão, planta com raiz	6611A110104	1
Klenk	Dente-de-Leão, planta com raiz	6611B130314	3
Klenk	Dente-de-Leão, planta com raiz	5122013b	1
Klenk	Dente-de-Leão, planta com raiz	6611B1104104	1
Klenk	Dente-de-Leão, planta com raiz	6611B090306	1
Klenk	Dente-de-Leão, planta com raiz	6611B-120620	1
Klenk	Dente-de-Leão, planta com raiz	6611B-131206	1
Klenk	Dente-de-Leão, planta com raiz	6611B110104	5
Klenk	Dente-de-Leão, planta com raiz	6611B110929	2
Bombastus	Dente-de-Leão, planta com raiz	277597	6
Phönix	Dente-de-Leão, planta com raiz	6611B130321	29
Sanacorp	Dente-de-Leão, planta com raiz	13108803	2
Caelo	Dente-de-Leão, planta com raiz	10121602	1
Caelo	Dente-de-Leão, planta sem raiz	11217107	1
Caelo	Dente-de-Leão, planta sem raiz	11030311	1
Caelo	Dente-de-Leão, planta sem raiz	11217109	2
Caelo	Dente-de-Leão, planta sem raiz	7031305	1
Caelo	Dente-de-Leão, planta sem raiz	11371904	2
Caelo	Dente-de-Leão, planta sem raiz	1127102	1
Caelo	Dente-de-Leão, planta sem raiz	13091305	1
Caelo	Dente-de-Leão, planta sem raiz	11371907	1
Caelo	Dente-de-Leão, planta sem raiz	11371902	1
Caelo	Dente-de-Leão, planta sem raiz	1137907	1
Caelo	Dente-de-Leão, planta sem raiz	9011403	1
Caelo	Dente-de-Leão, planta sem raiz	107063	1
Fagron	Dicloridrato de clorexidina	14A09B03	1
Fagron	Dicloridrato de clorexidina	14A09-B03-293425	1
Falcento	D-Ribose	201206712	2
Falcento	D-Ribose	201209702	1
Falcento	D-Ribose	JXCZSJ14-D-010	1
Unisan	D-Ribose	JXCZSJ13D-013	2

E

Supplier	Substance	Batch	Spectra
Caelo	Echinacea pallida	11115206	1
Caelo	Echinacea pallida	12244504	1
Bombastus	Endro, cortado	50836505	1
Caelo	Endro, cortado	11295109	1
Caelo	Endro, cortado	13007601	1
Caelo	Endro, cortado	13007605	1
Caelo	Endro, cortado	15178603	1
Caelo	Endro, cortado	13007602	1
Caelo	Endro, cortado	13007608	1
Klenk	Endro, cortado	3531B110726	1
Caelo	Epilobium angustifolium, planta	11347318	2
Caelo	Epilobium angustifolium, planta	11347311	1
Caelo	Epilobium angustifolium, planta	13104702	1
Caelo	Epilobium angustifolium, planta	11347316	1
Caelo	Epilobium angustifolium, planta	13200203	1
Caelo	Epilobium parviflorum	12064506	1
Bahnhof-Apotheke	Epilobium parviflorum	17-121107	1
Bombastus	Epilobium parviflorum	281846	2
Caelo	Epilobium parviflorum	7071201	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Epilobium parviflorum	9378908	1
Caelo	Epilobium parviflorum	29121201	1
Caelo	Epilobium parviflorum	2412E-01641	1
Caelo	Epilobium parviflorum	1031301	1
Caelo	Epilobium parviflorum	18031305	1
Caelo	Epilobium parviflorum	28031318	1
Caelo	Epilobium parviflorum	12041301	1
Caelo	Epilobium parviflorum	21061307	1
Caelo	Epilobium parviflorum	13071301	1
Caelo	Epilobium parviflorum	10326107	1
Caelo	Epilobium parviflorum	2081305	1
Caelo	Epilobium parviflorum	412041	1
Caelo	Epilobium parviflorum	16081302	1
Caelo	Epilobium parviflorum	16081304	1
Caelo	Epilobium parviflorum	15101302	1
Caelo	Epilobium parviflorum	13200203	7
Caelo	Epilobium parviflorum	31101303	1
Caelo	Epilobium parviflorum	15011411	1
Caelo	Epilobium parviflorum	13355906	2
Caelo	Epilobium parviflorum	14267909	1
Caelo	Epilobium parviflorum	10326104	5
Caelo	Epilobium parviflorum	13200201	3
Caelo	Epilobium parviflorum	13200202-3481312102	1
Caelo	Epilobium parviflorum	10326108	14
Caelo	Epilobium parviflorum	12117701-3371319012	1
Galke	Epilobium parviflorum	47502	1
Galke	Epilobium parviflorum	22347	4
Klenk	Epilobium parviflorum	4721C2120321	1
Hepart AG	Epilobium parviflorum	10326110	2
Klenk	Epilobium parviflorum	C120321	1
Klenk	Epilobium parviflorum	A120418	1
Klenk	Epilobium parviflorum	4721B130528	1
Klenk	Epilobium parviflorum	4721A101010	2
Klenk	Epilobium parviflorum	4721C120321	10
Klenk	Epilobium parviflorum	4721A120418	11
Klenk	Epilobium parviflorum	4721C110701	4
Klenk	Epilobium parviflorum	4721C130618	4
Klenk	Epilobium parviflorum	4721A120903	7
Klenk	Epilobium parviflorum	2512U-01641	1
Caelo	Epilobium parviflorum	12117701	8
Caelo	Erva Alchemilla alpina, cortada	12147202	3
Caelo	Erva Alchemilla alpina, cortada	12147205	2
Caelo	Erva Alchemilla alpina, cortada	12147203	1
Caelo	Erva Alchemilla alpina, cortada	1214204	1
Caelo	Erva Alchemilla alpina, cortada	12147203-3470312131	1
Caelo	Erva Alchemilla alpina, cortada	11063608	1
Caelo	Erva Alchemilla alpina, cortada	12147206	3
Alfred Galke	Erva bolsa-de-pastor	20591	1
Bahnhof-Apotheke	Erva bolsa-de-pastor	4-120924	1
Bombastus	Erva bolsa-de-pastor	269594	4
Bombastus	Erva bolsa-de-pastor	278856	2
Bombastus	Erva bolsa-de-pastor	269977	1
Bombastus	Erva bolsa-de-pastor	284136	1
Bombastus	Erva bolsa-de-pastor	12345	2
Bombastus	Erva bolsa-de-pastor	287350	1
Caelo	Erva bolsa-de-pastor	11036406	5
Caelo	Erva bolsa-de-pastor	14061201	1
Caelo	Erva bolsa-de-pastor	11091202	1
Caelo	Erva bolsa-de-pastor	15101202	1
Caelo	Erva bolsa-de-pastor	1132820111-14	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erva bolsa-de-pastor	11328203	5
Caelo	Erva bolsa-de-pastor	11328204	3
Caelo	Erva bolsa-de-pastor	269595	1
Caelo	Erva bolsa-de-pastor	12354201	11
Caelo	Erva bolsa-de-pastor	11328209	6
Caelo	Erva bolsa-de-pastor	11328205	1
Caelo	Erva bolsa-de-pastor	10061301	1
Caelo	Erva bolsa-de-pastor	12354202	2
Caelo	Erva bolsa-de-pastor	12354204	16
Caelo	Erva bolsa-de-pastor	12354203	13
Caelo	Erva bolsa-de-pastor	12354001	1
Caelo	Erva bolsa-de-pastor	3121301	1
Caelo	Erva bolsa-de-pastor	12354207	2
Caelo	Erva bolsa-de-pastor	12354209	1
Caelo	Erva bolsa-de-pastor	12354206	5
Caelo	Erva bolsa-de-pastor	11036401	1
Caelo	Erva bolsa-de-pastor	12354503	1
Caelo	Erva bolsa-de-pastor	11328201	6
Caelo	Erva bolsa-de-pastor	11328208	6
Caelo	Erva bolsa-de-pastor	12354203-3396310111	1
Caelo	Erva bolsa-de-pastor	11328207	8
Caelo	Erva bolsa-de-pastor	11328206	2
Caelo	Erva bolsa-de-pastor	12254202	1
Caelo	Erva bolsa-de-pastor	12354205	6
Caelo	Erva bolsa-de-pastor	11036404	1
Galke	Erva bolsa-de-pastor	21719	2
Galke	Erva bolsa-de-pastor	19483	1
Klenk	Erva bolsa-de-pastor	3671A-100414	2
Klenk	Erva bolsa-de-pastor	3671B111201	1
Klenk	Erva bolsa-de-pastor	B111201	1
Caelo	Erva bolsa-de-pastor	13344203	1
Caelo	Erva bolsa-de-pastor	11036410	2
Wolf	Erva bolsa-de-pastor	B449	2
an	Erva cardo-santo, cortada	13389704	1
Anzag	Erva cardo-santo, cortada	282281	1
Bombastus	Erva cardo-santo, cortada	271946	1
Caelo	Erva cardo-santo, cortada	9355208	1
Caelo	Erva cardo-santo, cortada	27111205	1
Caelo	Erva cardo-santo, cortada	10325402	5
Caelo	Erva cardo-santo, cortada	4743554	1
Caelo	Erva cardo-santo, cortada	13025901	5
Caelo	Erva cardo-santo, cortada	13025902	1
Caelo	Erva cardo-santo, cortada	12038202	1
Caelo	Erva cardo-santo, cortada	3091301	1
Caelo	Erva cardo-santo, cortada	13025903	3
Caelo	Erva cardo-santo, cortada	12038203	2
Caelo	Erva cardo-santo, cortada	10325404	1
Caelo	Erva cardo-santo, cortada	13389701	1
Gehe / 08.03.13 Redwood	Erva cardo-santo, cortada	205007	1
Klenk	Erva cardo-santo, cortada	A110517	1
Caelo	Erva Cytisus scoparius, cortada	11132209	1
Caelo	Erva Cytisus scoparius, cortada	4412Q-01680	1
Caelo	Erva Cytisus scoparius, cortada	12358802	1
Caelo	Erva Cytisus scoparius, cortada	12358804	3
Caelo	Erva Cytisus scoparius, cortada	12358805	1
Caelo	Erva Cytisus scoparius, cortada	13241601	1
Galke	Erva Cytisus scoparius, cortada	12358803	4
Phönix	Erva Cytisus scoparius, cortada	12358801	2
Kräuter Schulte	Erva de dríade-branca (Drya…	38970	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erva de Ransom	11182207	1
Caelo	Erva de Ransom	11182204	1
Caelo	Erva de Ransom	11182203	1
Caelo	Erva de Ransom	12380802	2
Caelo	Erva de Ransom	12380801	2
Caelo	Erva de Ransom	12380803	1
Caelo	Erva de Ransom	14343305	1
Klenk	Erva de Ransom	3511B111005	2
Klenk	Erva de Ransom	712914	1
Gehe	Erva Gelopsis, cortada	3911A130320	6
Klenk	Erva Gelopsis, cortada	3911A080409	1
Klenk	Erva Gelopsis, cortada	3911A130110	3
Klenk	Erva Gelopsis, cortada	3911A090219	2
Klenk	Erva Gelopsis, cortada	3911a130320	1
Caesar/Noweda	Erva Hepatica Americana, cortada	11254608	1
Caelo	Erva hissopo, cortada	11374304	1
Caelo	Erva hissopo, cortada	13143902	1
Caesar & Loretz/ Noweda	Erva hissopo, cortada	11374301	1
Galke	Erva hissopo, cortada	20939	1
Phönix	Erva hissopo, cortada	11374306	1
Sanacorp	Erva hissopo, cortada	11374303	2
Sanacorp	Erva hissopo, cortada	13336101	7
Caelo	Erva marroio-branco, cortada	1153803	1
Caelo	Erva marroio-branco, cortada	12231604	4
Caelo	Erva marroio-branco, cortada	313091	1
Caelo	Erva marroio-branco, cortada	13289109	1
Caelo	Erva marroio-branco, cortada	11253802	1
Caelo	Erva marroio-branco, cortada	12231603	1
Caelo	Erva marroio-branco, cortada	12231601	4
Caelo	Erva marroio-branco, cortada	11253803	1
Caelo	Erva marroio-branco, cortada	12231605	4
Klenk	Erva marroio-branco, cortada	4141A130110	1
Klenk	Erva marroio-branco, cortada	13289102	1
Noweda	Erva marroio-branco, cortada	4141A080513	1
Alfred Galke	Erva mil-folhas	19861	1
Anzag 12.11.12 ek:3,85	Erva mil-folhas	11280513	1
Bahnhof-Apotheke	Erva mil-folhas	7-121011	1
Bombastus	Erva mil-folhas	274610	2
Bombastus	Erva mil-folhas	276498	1
Bombastus	Erva mil-folhas	274284	1
Bombastus	Erva mil-folhas	15006702	1
Bombastus	Erva mil-folhas	275964	1
Caelo	Erva mil-folhas	10101205	1
Caelo	Erva mil-folhas	11218404	1
Caelo	Erva mil-folhas	11280517	1
Caelo	Erva mil-folhas	11280511	2
Caelo	Erva mil-folhas	11306301	1
Caelo	Erva mil-folhas	12338304	15
Caelo	Erva mil-folhas	12338305	7
Caelo	Erva mil-folhas	5021302	1
Caelo	Erva mil-folhas	12379602	9
Caelo	Erva mil-folhas	12379603	7
Caelo	Erva mil-folhas	12338311	2
Caelo	Erva mil-folhas	12041302	1
Caelo	Erva mil-folhas	16041302	1
Caelo	Erva mil-folhas	H-220313-1	1
Caelo	Erva mil-folhas	13029104	5
Caelo	Erva mil-folhas	29071301	1
Caelo	Erva mil-folhas	10081301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erva mil-folhas	13029106	10
Caelo	Erva mil-folhas	13029105	4
Caelo	Erva mil-folhas	9101311	1
Caelo	Erva mil-folhas	16102013E	1
Caelo	Erva mil-folhas	12379606	9
Caelo	Erva mil-folhas	9121304	1
Caelo	Erva mil-folhas	12379607	1
Caelo	Erva mil-folhas	8011421	1
Caelo	Erva mil-folhas	27011404	1
Caelo	Erva mil-folhas	13381810	1
Caelo	Erva mil-folhas	13381805	1
Caelo	Erva mil-folhas	14018503	2
Caelo	Erva mil-folhas	1408510	1
Caelo	Erva mil-folhas	15006713	1
Caelo	Erva mil-folhas	15006720	1
Caelo	Erva mil-folhas	15006708	1
Caelo	Erva mil-folhas	13029108	9
Caelo	Erva mil-folhas	12336306	1
Caelo	Erva mil-folhas	13029103	13
Caelo	Erva mil-folhas	11280514	2
Caelo	Erva mil-folhas	12338306-3358319071	1
Caelo	Erva mil-folhas	1309106	1
Caelo	Erva mil-folhas	11280512	9
Caelo	Erva mil-folhas	18304002	1
Caelo	Erva mil-folhas	18304016	1
Caelo	Erva mil-folhas	18088002	1
Caelo	Erva mil-folhas	18304013	1
Caelo	Erva mil-folhas	12338303	10
Caelo	Erva mil-folhas	12379601	9
Caelo	Erva mil-folhas	13029107-3418310182	1
Caelo	Erva mil-folhas	13029107-3436311151	1
Caelo	Erva mil-folhas	13381806	2
Caelo	Erva mil-folhas	130929105	1
Caesar & Lorenz	Erva mil-folhas	12379605	3
Caesar & Loretz Gm…	Erva mil-folhas	11306303	1
Caesar & Loretz Gm…	Erva mil-folhas	12338306	3
Fagron	Erva mil-folhas	3613M-0165	1
Galke	Erva mil-folhas	21295	2
Galke	Erva mil-folhas	22048	7
Galke	Erva mil-folhas	23318	1
Galke	Erva mil-folhas	23735	1
Gehe	Erva mil-folhas	1128503	1
Gehe	Erva mil-folhas	4181A111122	5
Gehe	Erva mil-folhas	279023	3
Klenk	Erva mil-folhas	15333007	1
Klenk	Erva mil-folhas	4181A101102	1
Klenk	Erva mil-folhas	4181A110111	16
Klenk	Erva mil-folhas	A130709	1
Klenk	Erva mil-folhas	4181A130710	1
Klenk	Erva mil-folhas	4181130709	1
Klenk	Erva mil-folhas	4181B130709	2
Klenk	Erva mil-folhas	4181a11011	1
Klenk	Erva mil-folhas	4181a130513	1
Klenk	Erva mil-folhas	4181A121130	12
nachprüfung	Erva mil-folhas	C1320	1
Noweda	Erva mil-folhas	12378603	1
Noweda	Erva mil-folhas	13381804	2
Phagron	Erva mil-folhas		3
Caelo	Erva mil-folhas	18088008	1
Phönix	Erva mil-folhas	4181A130513	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Wolf	Erva mil-folhas	230010	1
Wolf	Erva mil-folhas	B230010	9
Caelo	Erva trigo sarraceno, cortada	11212612	1
Caelo	Erva trigo sarraceno, cortada	11212808	2
Caelo	Erva trigo sarraceno, cortada	30041301	1
Caelo	Erva trigo sarraceno, cortada	2051303	1
Caelo	Erva trigo sarraceno, cortada	13051303	1
Caelo	Erva trigo sarraceno, cortada	11212809	1
Caelo	Erva trigo sarraceno, cortada	11212817	6
Caelo	Erva trigo sarraceno, cortada	11212807	2
Caelo	Erva trigo sarraceno, cortada	5111302	1
Caelo	Erva trigo sarraceno, cortada	11212810	1
Caelo	Erva trigo sarraceno, cortada	11212814	2
Caelo	Erva trigo sarraceno, cortada	13193203	1
Hepart AG	Erva trigo sarraceno, cortada	B120509	2
Klenk	Erva trigo sarraceno, cortada	4581B120509	3
Caelo	Erva trigo sarraceno, cortada	11212812	1
Caelo	Erva verga-de-ouro, europeia	13386908	1
Caelo	Erva verga-de-ouro, europeia	12343102	1
Caelo	Erva verga-de-ouro, europeia	12343103-3466312121	1
Klenk	Erva verga-de-ouro, europeia	1781B110706	1
Kenk / Phoenix	Erva verga-de-ouro, europeia	1781B110826	1
Sanacorp	Erva verga-de-ouro, europeia	12343103	1
Galke	Erva-benta, cortada	20881	1
Kräuter Schulte	Erva-benta, cortada	51737	1
Anzag 12.03.13 ek:…	Erva-de-são-joão	11185608	2
Caelo	Erva-de-são-joão	12092201	1
Aurica	Erva-de-são-joão	521200778	1
Aurica	Erva-de-são-joão	521202559	1
Bahnhof-Apotheke	Erva-de-são-joão	4-121018	1
Bombastus	Erva-de-são-joão	268913	1
Bombastus	Erva-de-são-joão	275106	6
Bombastus	Erva-de-são-joão	265761	1
Bombastus	Erva-de-são-joão	268834	2
Caelo	Erva-de-são-joão	4021B110321	1
Caelo	Erva-de-são-joão	11185602	1
Caelo	Erva-de-são-joão	11185608	18
Caelo	Erva-de-são-joão	5021301	1
Caelo	Erva-de-são-joão	1185608	1
Caelo	Erva-de-são-joão	16041301	1
Caelo	Erva-de-são-joão	12092204	1
Caelo	Erva-de-são-joão	13091303	1
Caelo	Erva-de-são-joão	111185608	1
Caelo	Erva-de-são-joão	11185607	1
Caelo	Erva-de-são-joão	30011401	1
Caelo	Erva-de-são-joão	132203204	1
Caelo	Erva-de-são-joão	15068105	1
Caelo	Erva-de-são-joão	268913	1
Caelo	Erva-de-são-joão	13203204	6
Caelo	Erva-de-são-joão	13203205	1
Finze	Erva-de-são-joão	9297303	1
Galke	Erva-de-são-joão	21034	1
Galke	Erva-de-são-joão	21990	4
Galke	Erva-de-são-joão	23054	1
Galke	Erva-de-são-joão	21556	1
Gehe	Erva-de-são-joão	9297305	1
Gehe	Erva-de-são-joão	11185602	1
Bombastus	Erva-de-são-joão	281530	1
Hepart AG	Erva-de-são-joão	B-445,kbA	1
Klenk	Erva-de-são-joão	15068103	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Erva-de-são-joão	4021A100819	1
Klenk	Erva-de-são-joão	4021A100819	21
Klenk	Erva-de-são-joão	4021A100819914	2
Klenk	Erva-de-são-joão	4021A100919	1
Klenk	Erva-de-são-joão	4021A-100819	1
Klenk	Erva-de-são-joão	A121120	1
Klenk	Erva-de-são-joão	4012A100819	1
Klenk	Erva-de-são-joão	A130612	3
Klenk	Erva-de-são-joão	4021A130612	4
Klenk	Erva-de-são-joão	4021a100819	1
Klenk	Erva-de-são-joão	4021a120604	1
Klenk	Erva-de-são-joão	4021B110321	2
Klenk	Erva-de-são-joão	4021A120604	16
Klenk	Erva-de-são-joão	4021A120905	9
Noweda	Erva-de-são-joão	12092202	6
Caelo	Erva-de-são-joão	12092209	2
Klenk	Erva-de-são-joão	4021A00819	1
Wolf	Erva-de-são-joão	206152	1
Wolf	Erva-de-são-joão	B206152	1
Wolf	Erva-de-são-joão	19468	2
Wolf	Erva-de-são-joão	B-455	2
Wolf	Erva-de-são-joão	B-424	1
Caelo	Erva-doce	311903	1
Fagron	Erva-doce	2870A130304	3
Fargron/Noweda	Erva-doce	2870A150810	1
Klenk	Erva-doce	2870A140528	2
Klenk	Erva-doce	2870130304A	1
Klenk	Erva-doce	2870A131002	1
AHD	Erva-doce, amarga	15006502	1
AHD;11.05.15;3,23	Erva-doce, amarga	14376408	3
Alfred Galke	Erva-doce, amarga	18270	1
Bahnhof-Apotheke	Erva-doce, amarga	11-121029	1
Bombastus	Erva-doce, amarga	268130	2
Bombastus	Erva-doce, amarga	285609	1
Bombastus	Erva-doce, amarga	296877	3
Bombastus	Erva-doce, amarga	307641	1
Bombastus	Erva-doce, amarga	299386	3
Bombastus	Erva-doce, amarga	289870	2
Bombastus	Erva-doce, amarga	299385	3
Bombastus	Erva-doce, amarga	280891	2
Bombastus	Erva-doce, amarga	289870	1
Bombastus	Erva-doce, amarga	289869	2
Bombastus	Erva-doce, amarga	293627	1
Bombastus	Erva-doce, amarga	275922	4
Cae	Erva-doce, amarga	Int.Ch.314090	1
Caelo	Erva-doce, amarga	16061202	1
Caelo	Erva-doce, amarga	11185501	1
Caelo	Erva-doce, amarga	6091201	1
Caelo	Erva-doce, amarga	12094703	2
Caelo	Erva-doce, amarga	1209474	1
Caelo	Erva-doce, amarga	12035102	2
Caelo	Erva-doce, amarga	27121201	1
Caelo	Erva-doce, amarga	12167102	4
Caelo	Erva-doce, amarga	11016330	1
Caelo	Erva-doce, amarga	402311545	1
Caelo	Erva-doce, amarga	12094710	4
Caelo	Erva-doce, amarga	12094712	4
Caelo	Erva-doce, amarga	12094716	8
Caelo	Erva-doce, amarga	7031306	1
Caelo	Erva-doce, amarga	13020802	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erva-doce, amarga	12094720	7
Caelo	Erva-doce, amarga	4061302	1
Caelo	Erva-doce, amarga	5061302	1
Caelo	Erva-doce, amarga	12094721	3
Caelo	Erva-doce, amarga	12094719	4
Caelo	Erva-doce, amarga	12094724	4
Caelo	Erva-doce, amarga	13200401	4
Caelo	Erva-doce, amarga	14111301	1
Caelo	Erva-doce, amarga	13148303	2
Caelo	Erva-doce, amarga	12362710	1
Caelo	Erva-doce, amarga	13148305	3
Caelo	Erva-doce, amarga	9121305	1
Caelo	Erva-doce, amarga	13200402	2
Caelo	Erva-doce, amarga	13148306	1
Caelo	Erva-doce, amarga	13371605	1
Caelo	Erva-doce, amarga	13371610	1
Caelo	Erva-doce, amarga	13371610	2
Caelo	Erva-doce, amarga	13398502	1
Caelo	Erva-doce, amarga	5121401	1
Caelo	Erva-doce, amarga	13398502	1
Caelo	Erva-doce, amarga	14376405	1
Caelo	Erva-doce, amarga	15006507	1
Caelo	Erva-doce, amarga	15443203	2
Caelo	Erva-doce, amarga	15443205	2
Caelo	Erva-doce, amarga	15443209	3
Caelo	Erva-doce, amarga	154443204	1
Caelo	Erva-doce, amarga	15443213	1
Caelo	Erva-doce, amarga	16298101	1
Caelo	Erva-doce, amarga	17341502	1
Caelo	Erva-doce, amarga	14255802	3
Caelo	Erva-doce, amarga	12167101	1
Caelo	Erva-doce, amarga	12094715	4
Caelo	Erva-doce, amarga	12345678	1
Caelo	Erva-doce, amarga	16005902	1
Caelo	Erva-doce, amarga	15007601	1
Caelo	Erva-doce, amarga	14376408;21S08	1
Caelo	Erva-doce, amarga	17341515	3
Caelo	Erva-doce, amarga	13148304	24
Caelo	Erva-doce, amarga	12094717	1
Caelo	Erva-doce, amarga	12035102	1
Caelo	Erva-doce, amarga	15443202	5
Caelo	Erva-doce, amarga	15443215	5
Caelo	Erva-doce, amarga	12094726	2
Caelo	Erva-doce, amarga	15141004	1
Caelo	Erva-doce, amarga	15443208	2
Caelo	Erva-doce, amarga	15443212	4
Caelo	Erva-doce, amarga	1302081	1
Caelo	Erva-doce, amarga	13020801	4
Caelo	Erva-doce, amarga	1320041	1
Caelo	Erva-doce, amarga	13148307	1
Caelo	Erva-doce, amarga	15006501	2
Caelo	Erva-doce, amarga	1S443206	1
Caelo	Erva-doce, amarga	14376406	2
Caelo	Erva-doce, amarga	15443216	2
Caelo	Erva-doce, amarga	19178804	2
Caelo	Erva-doce, amarga	14376402	1
Caelo	Erva-doce, amarga	15006508	3
Caelo	Erva-doce, amarga	15443204	8
Caelo	Erva-doce, amarga	17341503	1
Caelo	Erva-doce, amarga	17341510	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erva-doce, amarga	12094716-3408310191	1
Caelo	Erva-doce, amarga	13148304-3500411070	1
Caelo	Erva-doce, amarga	14376401	2
Caelo	Erva-doce, amarga	16298102	1
Caesar & Loretz Gm...	Erva-doce, amarga	11016331	1
Caesar & Loretz Gm...	Erva-doce, amarga	11016319	1
Caesar & Loretz Gm...	Erva-doce, amarga	12094705	4
Caesar & Loretz Gm...	Erva-doce, amarga	12094705	2
Caesar & Loretz Gm...	Erva-doce, amarga	12094707	6
Caesar & Loretz Gm...	Erva-doce, amarga	12094711	2
Caesar & Loretz Gm...	Erva-doce, amarga	12094725	8
Defektur	Erva-doce, amarga	7/13	1
Defektur	Erva-doce, amarga	52/13	1
Defektur	Erva-doce, amarga	57/13	1
Fagron	Erva-doce, amarga	1406211545	1
Fagron	Erva-doce, amarga		1
Fagron	Erva-doce, amarga	6858913	1
Gahlke	Erva-doce, amarga	20362	1
galke	Erva-doce, amarga	19938	3
Galke	Erva-doce, amarga	22176	1
GALKE	Erva-doce, amarga	27755	1
Gehe	Erva-doce, amarga	2860A120412	24
Caelo	Erva-doce, amarga	1250117/15443216	1
Hepart AG	Erva-doce, amarga	B492,kbA	1
K	Erva-doce, amarga	2860A160302	1
Klenk	Erva-doce, amarga	2860A110704	4
Klenk	Erva-doce, amarga	3812A-01545	1
Klenk	Erva-doce, amarga	2880N120418	4
Klenk	Erva-doce, amarga	2860A140224	1
Klenk	Erva-doce, amarga	2860A140612	18
Klenk	Erva-doce, amarga	2860A140224	1
Klenk	Erva-doce, amarga	2860A130513	2
Klenk	Erva-doce, amarga	2860A150320	21
Klenk	Erva-doce, amarga	2860A140613	3
Klenk	Erva-doce, amarga	2866B100211	1
Klenk	Erva-doce, amarga	2866B130206	1
Klenk	Erva-doce, amarga	2866B110318	1
Klenk	Erva-doce, amarga	2860A160606	1
Klenk	Erva-doce, amarga	2860,A150617	1
Klenk	Erva-doce, amarga	28060A140612	1
Klenk	Erva-doce, amarga	2860a-140224	1
Klenk	Erva-doce, amarga	2860a120412	3
Kottas	Erva-doce, amarga	P15301479	1
Lamotte / Sanacorp	Erva-doce, amarga	2860A150617	6
Noweda	Erva-doce, amarga	2860A180212	1
Noweda 06.04.2016	Erva-doce, amarga	15443201	1
Caelo	Erva-doce, amarga	12094704	4
Phönix	Erva-doce, amarga	12094708	2
Caelo	Erva-doce, amarga	2150317	1
Klenk	Erva-doce, amarga	2880A100503	2
Caelo	Erva-doce, amarga	15006506	1
Caelo	Erva-doce, amarga	17020603	1
siehe Protokoll (Galke)	Erva-doce, amarga	sieheProtokoll	2
Spangro/gepepharm	Erva-doce, amarga	15007602	2
Klenk	Erva-doce, amarga	2860A130226	8
Wolf	Erva-doce, amarga	B-362	1
Wolf	Erva-doce, amarga	B362	2
Wolf	Erva-doce, amarga	B-493	1
Wolf	Erva-doce, amarga	B-682	1
Wolf	Erva-doce, amarga	B382	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Wolf	Erva-doce, amarga	B492	1
Wolf	Erva-doce, amarga	B-492	5
Anzag	Estigma de milho	274920	1
Aurica/Phönix	Estigma de milho	520901387	1
Bahnhof-Apotheke	Estigma de milho	20-121018	1
Bombastus	Estigma de milho	282574	1
Bombastus	Estigma de milho	285912	1
Bombastus	Estigma de milho	276776	1
Bombastus	Estigma de milho	81113a	1
Bombastus	Estigma de milho	17001482	1
Bombastus	Estigma de milho	19002817	1
Caelo	Estigma de milho	10325902	2
Caelo	Estigma de milho	10325906	7
Caelo	Estigma de milho	10325904	1
Caelo	Estigma de milho	10325907	4
Caelo	Estigma de milho	10325905	1
Caelo	Estigma de milho	280363	1
Caelo	Estigma de milho	11280404	2
Caelo	Estigma de milho	13277201	1
Caelo	Estigma de milho	13277202	1
Caelo	Estigma de milho	13277207	1
Caelo	Estigma de milho	11280405	11
Caelo	Estigma de milho	13277205	1
Caelo	Estigma de milho	15226102	1
Caelo	Estigma de milho	15226103	1
Gehe	Estigma de milho	18041004	1
Klenk	Estigma de milho	5581A081204	1
Klenk	Estigma de milho	5581A111206	1
Klenk	Estigma de milho	A110411	1
Richter	Estigma de milho	B189316	1
Sana 21.10.14 Ek 3.57	Estigma de milho	13381603	2
Caelo	Estróbilo de lúpulo	13123802	9
Bombaltus	Estróbilo de lúpulo	274724	1
Bombastus	Estróbilo de lúpulo	276976	1
Bombastus	Estróbilo de lúpulo	271870	1
Bombastus	Estróbilo de lúpulo	208502	1
Caelo	Estróbilo de lúpulo	15061211	1
Caelo	Estróbilo de lúpulo	12008307	2
Caelo	Estróbilo de lúpulo	1451b120817	1
Caelo	Estróbilo de lúpulo	5021306	1
Caelo	Estróbilo de lúpulo	12008317	6
Caelo	Estróbilo de lúpulo	12380101	6
Caelo	Estróbilo de lúpulo	12380103	2
Caelo	Estróbilo de lúpulo	1451B130107	6
Caelo	Estróbilo de lúpulo	6091303	1
Caelo	Estróbilo de lúpulo	13123803	9
Caelo	Estróbilo de lúpulo	12221807	1
Caelo	Estróbilo de lúpulo	13123902	1
Caelo	Estróbilo de lúpulo	4111304	1
Caelo	Estróbilo de lúpulo	13123807	1
Caelo	Estróbilo de lúpulo	30121301	1
Caelo	Estróbilo de lúpulo	13123803	1
Caelo	Estróbilo de lúpulo	13123804	3
Caelo	Estróbilo de lúpulo	131223805	1
Caelo	Estróbilo de lúpulo	14068007	1
Caelo	Estróbilo de lúpulo	12221804	1
Caelo	Estróbilo de lúpulo	12008302	1
Caelo	Estróbilo de lúpulo	12008315	1
Caelo	Estróbilo de lúpulo	4756769	1
Caelo	Estróbilo de lúpulo	12008309	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estróbilo de lúpulo	10240308	1
Caelo	Estróbilo de lúpulo	13187602	1
Caelo	Estróbilo de lúpulo	12008305	1
Caelo	Estróbilo de lúpulo	120008312	1
Caelo	Estróbilo de lúpulo	12221805	3
Caelo	Estróbilo de lúpulo	12221802	2
Caelo	Estróbilo de lúpulo	12092001	2
Caelo	Estróbilo de lúpulo	12008310	3
Caelo	Estróbilo de lúpulo	12008310	3
Caelo	Estróbilo de lúpulo	12006305	1
Caelo	Estróbilo de lúpulo	12008313	2
Caelo	Estróbilo de lúpulo	12008317	1
Caelo	Estróbilo de lúpulo	13123803-3505411011	1
Caelo	Estróbilo de lúpulo	13123804-3563412081	1
Galke	Estróbilo de lúpulo	20928	3
Galke	Estróbilo de lúpulo	20928	2
Galke	Estróbilo de lúpulo	23363	1
Caelo	Estróbilo de lúpulo	13123806	1
Klenk	Estróbilo de lúpulo	1451B120202	6
Klenk	Estróbilo de lúpulo	1451B111004	1
Klenk	Estróbilo de lúpulo	20071301	1
Klenk	Estróbilo de lúpulo	B130409	1
Klenk	Estróbilo de lúpulo	1451b130409	1
Klenk	Estróbilo de lúpulo	1451B140408	1
Klenk	Estróbilo de lúpulo	1450A110712	1
Klenk	Estróbilo de lúpulo	1451B130409	1
Klenk	Estróbilo de lúpulo	1451b130107	1
Klenk	Estróbilo de lúpulo	1451B130409	9
Klenk	Estróbilo de lúpulo	1451B-120817	1
Klenk	Estróbilo de lúpulo	1451B120817	7
Noweda	Estróbilo de lúpulo	274725	1
Caelo	Estróbilo de lúpulo	13123802	3
Bombastus	Eufrásia	274553	1
Bombastus	Eufrásia	270726	2
Bombastus	Eufrásia	278108	2
Bombastus	Eufrásia	277846	1
Caelo	Eufrásia	112211643	1
Caelo	Eufrásia	11030810	1
Caelo	Eufrásia	29011302	1
Caelo	Eufrásia	12103202	9
Caelo	Eufrásia	12103203	10
Caelo	Eufrásia	7051302	1
Caelo	Eufrásia	312052	1
Caelo	Eufrásia	13180001	5
Caelo	Eufrásia	30101307	1
Caelo	Eufrásia	13180004	5
Caelo	Eufrásia	12103201	1
Caelo	Eufrásia	13180005	2
Caelo	Eufrásia	8011419	1
Caelo	Eufrásia	13180008	1
Caelo	Eufrásia	14019107	1
Caelo	Eufrásia	1213202	1
Caelo	Eufrásia	14019102	2
Caelo	Eufrásia	13180002	5
Caelo	Eufrásia	11030812	4
Galke	Eufrásia	20262	2
Klenk	Eufrásia	15029806	1
Klenk	Eufrásia	B101206	1
Klenk	Eufrásia	B130430	1
Klenk	Eufrásia	3871B130430	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Eufrásia	11030811	3
Euro OTC	Extrato de olíbano 80%	1104005V-04	2
Euro OTC	Extrato de olíbano 80%	1705033-01	1

F

Supplier	Substance	Batch	Spectra
Aurica/Phönix	Feijão, cascas	5052301	1
Bombastus	Feijão, cascas	272781	3
Bombastus	Feijão, cascas	278686	1
Bombastus	Feijão, cascas	282475	1
Bombastus	Feijão, cascas	278696	2
Bombastus	Feijão, cascas	270517	1
Bombastus	Feijão, cascas	240503	1
Cae	Feijão, cascas	Int.Ch.313011	1
Caelo	Feijão, cascas	29091201	1
Caelo	Feijão, cascas	8301004	1
Caelo	Feijão, cascas	6031301	1
Caelo	Feijão, cascas	11030604	6
Caelo	Feijão, cascas	1103061	1
Caelo	Feijão, cascas	11030601	1
Caelo	Feijão, cascas	13333801	1
Caelo	Feijão, cascas	1333802	1
Caelo	Feijão, cascas	13333803	1
Caelo	Feijão, cascas	14080002	1
Caelo	Feijão, cascas	15060905	1
Caelo	Feijão, cascas	12358703	5
Caelo	Feijão, cascas	10006507	1
Caelo	Feijão, cascas	11233603	1
Caelo	Feijão, cascas	11030602	5
Caelo	Feijão, cascas	11030605	1
Galke	Feijão, cascas	21219	1
Klenk	Feijão, cascas	671A100816	2
Klenk	Feijão, cascas	171A110301	1
Klenk	Feijão, cascas	C120321	2
Klenk	Feijão, cascas	671C121105	8
Klenk	Feijão, cascas	C121105	2
Klenk	Feijão, cascas	671C130620	6
Klenk	Feijão, cascas	C130620	1
Klenk	Feijão, cascas	671A110420	9
Klenk	Feijão, cascas	671B180726	1
Klenk	Feijão, cascas	671A180925	1
Klenk	Feijão, cascas	671A-110420	1
Klenk	Feijão, cascas	671A110301	1
Klenk	Feijão, cascas	671C120321	16
Apofit	Feno-grego	222392	1
Caelo	Feno-grego	12252601	2
Caelo	Feno-grego	11313203	1
Caelo	Feno-grego	13013801	1
Caelo	Feno-grego	1131206	1
Caelo	Feno-grego	12252603	3
Caelo	Feno-grego	13013803	6
Caelo	Feno-grego	13013805	3
Gehe	Feno-grego	11313204	1
Gehe	Feno-grego	13013811	2
Klenk	Feno-grego	7260A130603	3
Klenk	Feno-grego	9011301	1
Klenk	Feno-grego	A120118	2
Klenk	Feno-grego	8061301	1
Klenk	Feno-grego	A130603	1
Klenk	Feno-grego	7260A110530	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Feno-grego	7260A120118	2
Phoenix	Feno-grego	11313206	7
Caelo	Feno-grego	12252602	2
Caelo	Feno-grego pulverizado	12149605	1
Caelo	Feno-grego pulverizado	12149607	1
Caelo	Feno-grego pulverizado	13398302	1
Caelo	Feno-grego pulverizado	15308703	2
Caelo	Feno-grego pulverizado	7264a110201	2
Caelo	Feno-grego pulverizado	15120506	1
Caelo	Feno-grego pulverizado	14057807	1
Caelo	Feno-grego pulverizado	15308704	1
Caelo	Feno-grego pulverizado	14377201	2
Caelo	Feno-grego pulverizado	14057801	1
Fagron	Feno-grego pulverizado	12149603	1
Ichthyol/Phoenix	Feno-grego pulverizado	14377205	1
Klenk	Feno-grego pulverizado	A110201	1
Klenk	Feno-grego pulverizado	12082014A	1
Klenk	Feno-grego pulverizado	7264A110201	9
Klenk	Feno-grego pulverizado	7264B150303	1
Nachprüfung	Feno-grego pulverizado	2412E02239	1
Caelo	Fenol	11163801	1
Caelo	Fenol	11163809	1
Caelo	Fenol	7061305	1
Caelo	Fenol	12223014	1
Caelo	Fenol	12223020	1
Caelo	Fenol	12223022	1
Caelo	Fenol	12223001	1
-	Filipenda ulmaria	1511M-01685	1
-	Filipenda ulmaria	130849	1
Anzag	Filipenda ulmaria	10381604	5
Caelo	Filipenda ulmaria	10381602	3
Caelo	Filipenda ulmaria	10381601	1
Caelo	Filipenda ulmaria	12188704	2
Caelo	Filipenda ulmaria	12188703	1
Caelo	Filipenda ulmaria	12188803	10
Caelo	Filipenda ulmaria	4912E-01685	1
Caelo	Filipenda ulmaria	12188801	1
Caelo	Filipenda ulmaria	12188807	1
Caelo	Filipenda ulmaria	12188702	1
Caelo	Filipenda ulmaria	12188805	13
Caelo	Filipenda ulmaria	12188806	3
Caelo	Filipenda ulmaria	62487517	1
Galke	Filipenda ulmaria	20358	1
Sanacorp	Filipenda ulmaria	4541A120313	2
Weltecke	Filipenda ulmaria	67010413	1
Caelo	Flor de abrunheiro	12178101	2
Caelo	Flor de abrunheiro	11206906	1
Caelo	Flor de abrunheiro	12178104	4
Caelo	Flor de abrunheiro	12178105	1
Caelo	Flor de abrunheiro	12178102	9
Caelo	Flor de abrunheiro	12178103	2
Klenk	Flor de abrunheiro	2612E-01468	1
Caelo	Flor de abrunheiro, desinte…	1150N101109	2
Klenk	Flor de abrunheiro, desinte…	N101109	2
Klenk	Flor de abrunheiro, desinte…	1150n101109	1
Kräuter Schulte	Flor de abrunheiro, desinte…	53233	2
Caelo	Flor de arnica	10207405	1
Caelo	Flor de arnica	28071201	1
Caelo	Flor de arnica	10081204	1
Caelo	Flor de arnica	11259804	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de arnica	12227202	1
Caelo	Flor de arnica	122227202	1
Caelo	Flor de arnica	IntCh:212032	1
Caelo	Flor de arnica	11285705	1
Caelo	Flor de arnica	11259803	1
Caelo	Flor de arnica	11285703	1
Caelo	Flor de arnica	6112013A	1
Caelo	Flor de arnica	12227203	1
Caelo	Flor de arnica	1222702	1
Caelo	Flor de arnica	11374105	1
Caelo	Flor de arnica	11374103	1
Caelo	Flor de arnica	11374101	2
Caelo	Flor de arnica	11374102	2
Gehe	Flor de arnica	11259801	2
Klenk	Flor de arnica	1181B130605	1
Bombastus	Flor de calêndula	268626	1
Caelo	Flor de calêndula	12221706	2
Caelo	Flor de calêndula	13235503	3
Caelo	Flor de calêndula	15291501	1
Caelo	Flor de calêndula	12221710	1
Caelo	Flor de calêndula	12221705	1
Caelo	Flor de calêndula	12221511	1
Caelo	Flor de calêndula	12221508	1
Caelo	Flor de calêndula	122221707	1
Caelo	Flor de calêndula	12221708	3
Caelo	Flor de calêndula	12221510-3356319071	1
Caelo	Flor de calêndula	12221510-3435311151	1
Caelo	Flor de calêndula	13235502	3
galke,	Flor de calêndula	12028	1
Bombastus	Flor de calêndula	280306	1
Klenk	Flor de calêndula	1250A110511	1
Klenk	Flor de calêndula	C120321	1
Klenk	Flor de calêndula	1241B120312	1
Klenk	Flor de calêndula	1241B130517	1
Wolf	Flor de calêndula	23342	1
Anzag	Flor de calêndula, cortada	12221706	12
Bahnhof-Apotheke	Flor de calêndula, cortada	17-121106	1
Bombastus	Flor de calêndula, cortada	270046	1
Bombastus	Flor de calêndula, cortada	253620	1
Bombastus	Flor de calêndula, cortada	279632	1
Bombastus	Flor de calêndula, cortada	275813	1
Bombastus	Flor de calêndula, cortada	275128	1
Bombastus	Flor de calêndula, cortada	207294	1
Bombastus	Flor de calêndula, cortada	234997	1
Caelo	Flor de calêndula, cortada	13235502	9
Caelo	Flor de calêndula, cortada	295556	1
Caelo	Flor de calêndula, cortada	22061203	1
Caelo	Flor de calêndula, cortada	12071201	1
Caelo	Flor de calêndula, cortada	11187612	12
Caelo	Flor de calêndula, cortada	11187610	3
Caelo	Flor de calêndula, cortada	27101201	1
Caelo	Flor de calêndula, cortada	19111206	1
Caelo	Flor de calêndula, cortada	11187611	3
Caelo	Flor de calêndula, cortada	31121202	1
Caelo	Flor de calêndula, cortada	5021305	1
Caelo	Flor de calêndula, cortada	12221705	4
Caelo	Flor de calêndula, cortada	11221407	1
Caelo	Flor de calêndula, cortada	12221704	13
Caelo	Flor de calêndula, cortada	8041302	1
Caelo	Flor de calêndula, cortada	3061301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de calêndula, cortada	12221707	2
Caelo	Flor de calêndula, cortada	21091301	1
Caelo	Flor de calêndula, cortada	12221710	2
Caelo	Flor de calêndula, cortada	9112013C	1
Caelo	Flor de calêndula, cortada	13235501	4
Caelo	Flor de calêndula, cortada	9121303	1
Caelo	Flor de calêndula, cortada	18121301	1
Caelo	Flor de calêndula, cortada	13235505	1
Caelo	Flor de calêndula, cortada	13410202	2
Caelo	Flor de calêndula, cortada	15040301	1
Caelo	Flor de calêndula, cortada	10291904	1
Caelo	Flor de calêndula, cortada	12221701	1
Caelo	Flor de calêndula, cortada	122221704	1
Caelo	Flor de calêndula, cortada	1187612	2
Caelo	Flor de calêndula, cortada	12221708	11
Caelo	Flor de calêndula, cortada	13235506	2
Caelo	Flor de calêndula, cortada	AKD1	1
Caelo	Flor de calêndula, cortada	1325502	1
Gehe	Flor de calêndula, cortada	260205	1
Klenk	Flor de calêndula, cortada	1241B130517	6
Klenk	Flor de calêndula, cortada	1241B150902	1
Klenk	Flor de calêndula, cortada	1241N151209	1
Klenk	Flor de calêndula, cortada	1241B160530	1
Klenk	Flor de calêndula, cortada	1241B120419	2
Klenk	Flor de calêndula, cortada	112211448	1
Klenk	Flor de calêndula, cortada	1240A110418	1
Klenk	Flor de calêndula, cortada	204311448	1
Klenk	Flor de calêndula, cortada	1241B130321	5
Klenk	Flor de calêndula, cortada	3013E1448	1
Klenk	Flor de calêndula, cortada	B130517	2
Klenk	Flor de calêndula, cortada	1241B140211	1
Klenk	Flor de calêndula, cortada	1241B130927	1
Klenk	Flor de calêndula, cortada	1241B110118	2
Noweda	Flor de calêndula, cortada	12221709	9
Klenk	Flor de calêndula, cortada	1241C120321	4
Fagron	Flor de calêndula, cortada	1241B120312	4
Sanacorp	Flor de calêndula, cortada	12221601	4
Caelo	Flor de calêndula, cortada	12221502	2
Klenk	Flor de camomila-vulgar	1290A-120620	1
Bahnhof-Apotheke	Flor de camomila-vulgar	11-121024	1
Bombastus	Flor de camomila-vulgar	268712	1
Bombastus	Flor de camomila-vulgar	274106	1
Bombastus	Flor de camomila-vulgar	273667	1
Bombastus	Flor de camomila-vulgar	276095	5
Bombastus	Flor de camomila-vulgar	276307	1
Bombastus	Flor de camomila-vulgar	271781	1
Bombastus	Flor de camomila-vulgar	281103	2
Bombastus	Flor de camomila-vulgar	287855	1
Bombastus	Flor de camomila-vulgar	299185	1
Bombastus	Flor de camomila-vulgar	283710	2
Bombastus	Flor de camomila-vulgar	274105	1
Bombastus	Flor de camomila-vulgar	273388	1
Bombastus	Flor de camomila-vulgar	277997	1
Bombastus	Flor de camomila-vulgar	265419	1
Bombastus	Flor de camomila-vulgar	268408	1
Bombastus	Flor de camomila-vulgar	268408	1
Bombastus	Flor de camomila-vulgar	292757	1
Bombastus	Flor de camomila-vulgar	277959	2
Bombastus	Flor de camomila-vulgar	264997	1
Caelo	Flor de camomila-vulgar	12294802	15

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de camomila-vulgar	12294804	1
Caelo	Flor de camomila-vulgar	11169607	1
Caelo	Flor de camomila-vulgar	13061201	1
Caelo	Flor de camomila-vulgar	10081201	1
Caelo	Flor de camomila-vulgar	22081202	1
Caelo	Flor de camomila-vulgar	12059606	2
Caelo	Flor de camomila-vulgar	5081201	1
Caelo	Flor de camomila-vulgar	12244802	4
Caelo	Flor de camomila-vulgar	27091203	1
Caelo	Flor de camomila-vulgar	11214810	1
Caelo	Flor de camomila-vulgar	11101203	1
Caelo	Flor de camomila-vulgar	17101204	1
Caelo	Flor de camomila-vulgar	12244803	3
Caelo	Flor de camomila-vulgar	12111903	2
Caelo	Flor de camomila-vulgar	13111201	1
Caelo	Flor de camomila-vulgar	16111202	1
Caelo	Flor de camomila-vulgar	19111207	1
Caelo	Flor de camomila-vulgar	22111201	1
Caelo	Flor de camomila-vulgar	22111202	1
Caelo	Flor de camomila-vulgar	12299701	1
Caelo	Flor de camomila-vulgar	22011303	1
Caelo	Flor de camomila-vulgar	12299703	2
Caelo	Flor de camomila-vulgar	20021313	1
Caelo	Flor de camomila-vulgar	13031306	1
Caelo	Flor de camomila-vulgar	19041306	1
Caelo	Flor de camomila-vulgar	12361701	3
Caelo	Flor de camomila-vulgar	12337605	2
Caelo	Flor de camomila-vulgar	13014501	1
Caelo	Flor de camomila-vulgar	12337601	1
Caelo	Flor de camomila-vulgar	IntCh:313011	1
Caelo	Flor de camomila-vulgar	26081303	1
Caelo	Flor de camomila-vulgar	12337610	1
Caelo	Flor de camomila-vulgar	12361704	1
Caelo	Flor de camomila-vulgar	12337608	1
Caelo	Flor de camomila-vulgar	12361707	2
Caelo	Flor de camomila-vulgar	13210901	3
Caelo	Flor de camomila-vulgar	12361706	1
Caelo	Flor de camomila-vulgar	13011406	1
Caelo	Flor de camomila-vulgar	13288405	3
Caelo	Flor de camomila-vulgar	14276804	3
Caelo	Flor de camomila-vulgar	15090003	2
Caelo	Flor de camomila-vulgar	15258504	1
Caelo	Flor de camomila-vulgar	15258505	1
Caelo	Flor de camomila-vulgar	11218501	1
Caelo	Flor de camomila-vulgar	13210906	1
Caelo	Flor de camomila-vulgar	12361702	6
Caelo	Flor de camomila-vulgar	12361707	4
Caelo	Flor de camomila-vulgar	13210905	3
Caelo	Flor de camomila-vulgar	17338903	1
Caelo	Flor de camomila-vulgar	18290002	1
Caelo	Flor de camomila-vulgar	12244803	1
Caelo	Flor de camomila-vulgar	13210901-3478312171	1
Caelo	Flor de camomila-vulgar	12337607	2
Caelo	Flor de camomila-vulgar	12244805	4
Caelo	Flor de camomila-vulgar	12244804	2
Caelo	Flor de camomila-vulgar	12361706	3
Caelo	Flor de camomila-vulgar	13210905	1
Caelo	Flor de camomila-vulgar	18193705	1
Caelo	Flor de camomila-vulgar	13210903	1
Caelo	Flor de camomila-vulgar	13210901-3546411013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de camomila-vulgar	AKD5	1
Defektur	Flor de camomila-vulgar	56/12	1
Defektur	Flor de camomila-vulgar	10/13	1
Defektur	Flor de camomila-vulgar	29/13	1
Defektur	Flor de camomila-vulgar	59/13	1
Fagron	Flor de camomila-vulgar		1
Finze	Flor de camomila-vulgar	1290B101122	1
Finze	Flor de camomila-vulgar	12361703	6
Galke	Flor de camomila-vulgar	18471	5
Galke	Flor de camomila-vulgar	18803	1
Galke	Flor de camomila-vulgar	21652	1
Gehe	Flor de camomila-vulgar	11214802	1
Gehe	Flor de camomila-vulgar	11255204	1
Gehe	Flor de camomila-vulgar	12133009	1
Hepart AG	Flor de camomila-vulgar	B-477,kbA	1
Klenk	Flor de camomila-vulgar	1290B140123	2
k	Flor de camomila-vulgar	1290A140513	1
Klenk	Flor de camomila-vulgar	1290A150618	1
Klenk	Flor de camomila-vulgar	1290A20404	1
Klenk	Flor de camomila-vulgar	1290A120404	1
Klenk	Flor de camomila-vulgar	1290A120404	6
Klenk	Flor de camomila-vulgar	2310211452	1
Klenk	Flor de camomila-vulgar	27111204	1
Klenk	Flor de camomila-vulgar	1290A120403	3
Klenk	Flor de camomila-vulgar	1290A12061	1
Klenk	Flor de camomila-vulgar	1290A110825	1
Klenk	Flor de camomila-vulgar	1290B130415	39
Klenk	Flor de camomila-vulgar	1290A120601	2
Klenk	Flor de camomila-vulgar	B130415	2
Klenk	Flor de camomila-vulgar	11101302	1
Klenk	Flor de camomila-vulgar	14111314	1
Klenk	Flor de camomila-vulgar	A130502	1
Klenk	Flor de camomila-vulgar	A130516	1
Klenk	Flor de camomila-vulgar	A120529	1
Klenk	Flor de camomila-vulgar	16121301	1
Klenk	Flor de camomila-vulgar	1290A130516	3
Klenk	Flor de camomila-vulgar	1290A130502	1
Klenk	Flor de camomila-vulgar	1290A130516	9
Klenk	Flor de camomila-vulgar	A120529	1
Klenk	Flor de camomila-vulgar	1290A130502	1
Klenk	Flor de camomila-vulgar	1290B140624	1
Klenk	Flor de camomila-vulgar	1290A140508	1
Klenk	Flor de camomila-vulgar	1290A120620	13
Klenk	Flor de camomila-vulgar	1290A120529	1
Klenk	Flor de camomila-vulgar	4100113002	2
Klenk	Flor de camomila-vulgar	1290A120601	14
Klenk	Flor de camomila-vulgar	1290A180709	1
Klenk	Flor de camomila-vulgar	1290A110421	1
Klenk	Flor de camomila-vulgar	1290B130415	3
Klenk	Flor de camomila-vulgar	1290a120620	1
Klenk	Flor de camomila-vulgar	1290A110607	1
Klenk	Flor de camomila-vulgar	1290A120529	5
Phönix	Flor de camomila-vulgar	1300A120426	1
Sanacorp	Flor de camomila-vulgar	12294804	6
Sanacorp	Flor de camomila-vulgar	12294809	3
Sanacorp	Flor de camomila-vulgar	1300A120725	2
Sanacorp	Flor de camomila-vulgar	1290B140123	2
Spangropharm	Flor de camomila-vulgar	11169606	1
Wolf	Flor de camomila-vulgar	23242	1
Galke	Flor de castanha-da-índia, …	2614	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Flor de castanha-da-índia, …	1440A110311	3
Richter	Flor de castanha-da-índia, …	s-09/09	1
Apofit	Flor de centáurea	278776	1
Bombastus	Flor de centáurea	275759	2
Bombastus	Flor de centáurea	284030	1
Caelo	Flor de centáurea	11059209	2
Caelo	Flor de centáurea	12060203	4
Caelo	Flor de centáurea	12232501	2
Caelo	Flor de centáurea	12060202	2
Caelo	Flor de centáurea	14323302	1
Caelo	Flor de centáurea	15206601	1
Caelo	Flor de centáurea	72767368	1
Caelo	Flor de centáurea	12060205	4
Caelo	Flor de centáurea	11059206	2
Caelo	Flor de centáurea	11059211	2
Galke	Flor de centáurea	23131	2
Klenk	Flor de centáurea		1
Alliance	Flor de espinheiro-branco	13010403	1
Caelo	Flor de espinheiro-branco	13010403	5
Caelo	Flor de espinheiro-branco	7121201	1
Caelo	Flor de espinheiro-branco	11068208	1
Caelo	Flor de espinheiro-branco	11068206	1
Caelo	Flor de espinheiro-branco	13010402	2
Caelo	Flor de espinheiro-branco	11068209	1
Caelo	Flor de espinheiro-branco	13010402	3
Caelo	Flor de espinheiro-branco	11068202	1
Caelo	Flor de espinheiro-branco	21051301	1
Caelo	Flor de espinheiro-branco	25101301	1
Caelo	Flor de espinheiro-branco	13253303	1
Caelo	Flor de espinheiro-branco	13253304	1
Caelo	Flor de espinheiro-branco	1351B130819	3
Caesar & Loretz GmbH	Flor de espinheiro-branco	11068206	3
Hepart AG	Flor de espinheiro-branco	13010401	1
Klenk	Flor de espinheiro-branco	1351B111207	4
Klenk	Flor de espinheiro-branco	B1112107	1
an	Flor de hibisco	14018101	1
Caelo	Flor de hibisco	12267502	4
Caelo	Flor de hibisco	11036504	1
Caelo	Flor de hibisco	11036512	1
Caelo	Flor de hibisco	7121301	1
Caelo	Flor de hibisco	12267507	2
Caelo	Flor de hibisco	12267504	3
Caelo	Flor de hibisco	12007306	1
Caelo	Flor de hibisco	11036509	2
Caelo	Flor de hibisco	12267503	2
Caelo	Flor de hibisco	12267501	3
Caelo	Flor de hibisco	12267502	3
Caelo	Flor de hibisco	12267504	1
Caelo	Flor de hibisco	12267504-3428311150	1
Caelo	Flor de hibisco	11036511	1
Klenk	Flor de hibisco	1431B130205	1
Klenk	Flor de hibisco	B130205	1
Klenk	Flor de hibisco	1431B-110519	1
Klenk	Flor de hibisco	1431B131015	2
Klenk	Flor de hibisco	1431B111122	1
Sanacorp	Flor de hibisco	12267508	2
vedono	Flor de hibisco	12007313	1
Caelo	Flor de hibisco, cortada	13040402	1
Caelo	Flor de hibisco, cortada	13040401	2
Caelo	Flor de hibisco, cortada	10244507	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de jasmim	12143203	3
Klenk	Flor de jasmim	1460A110505	1
Phönix	Flor de jasmim	12143206	1
Anzag	Flor de lavanda	1488A12803	1
Bombastus	Flor de lavanda	268832	1
Bombastus	Flor de lavanda	274469	1
Bombastus	Flor de lavanda	279213	1
Caelo	Flor de lavanda	11054104	2
Caelo	Flor de lavanda	15061201	1
Caelo	Flor de lavanda	15061209	1
Caelo	Flor de lavanda	11327903	6
Caelo	Flor de lavanda	11327905	2
Caelo	Flor de lavanda	27091202	1
Caelo	Flor de lavanda	12088002	4
Caelo	Flor de lavanda	12088003	8
Caelo	Flor de lavanda	12031302	1
Caelo	Flor de lavanda	12088005	3
Caelo	Flor de lavanda	19071303	1
Caelo	Flor de lavanda	6091304	1
Caelo	Flor de lavanda	13185002	1
Caelo	Flor de lavanda	13159601	1
Caelo	Flor de lavanda	13336008	1
Caelo	Flor de lavanda	13387204	1
Caelo	Flor de lavanda	11054107	1
Caelo	Flor de lavanda	11054106	2
Caelo	Flor de lavanda	12088006	3
Caelo	Flor de lavanda	1318501	1
Caelo	Flor de lavanda	13185001-3389311070	1
Caelo	Flor de lavanda	13185001-3415310152	1
Caelo	Flor de lavanda	13185006	1
Caelo	Flor de lavanda	13185001	28
Fagron	Flor de lavanda	1489A120919	6
Galke	Flor de lavanda	21416	2
Hepart AG	Flor de lavanda	A130214	4
Herbasinica	Flor de lavanda	1488A130830	1
Caelo	Flor de lavanda	13185003	10
Klenk	Flor de lavanda	1489A1203	1
Klenk	Flor de lavanda	1488A111201	2
Klenk	Flor de lavanda	1488A120803	3
Klenk	Flor de lavanda	1488B130604	5
Klenk	Flor de lavanda	313U-01462	1
Klenk	Flor de lavanda	1489A100125	1
Klenk	Flor de lavanda	1489A120103	19
Klenk	Flor de lavanda	1489A130214	16
Klenk	Flor de lavanda	1488B130111	2
Bombastus	Flor de malva	273803	1
Bombastus	Flor de malva	13267304	1
Caelo	Flor de malva	20061201	1
Caelo	Flor de malva	10357902	1
Caelo	Flor de malva	11040106	4
Caelo	Flor de malva	8121202	1
Caelo	Flor de malva	27021301	1
Caelo	Flor de malva	12187405	4
Caelo	Flor de malva	12187404	4
Caelo	Flor de malva	12187501	6
Caelo	Flor de malva	12187502	1
Caelo	Flor de malva	13040402	1
Caelo	Flor de malva	18111303	1
Caelo	Flor de malva	13267303	2
Caelo	Flor de malva	13267302	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de malva	13351309	1
Caelo	Flor de malva	13351307	1
Caelo	Flor de malva	10357904	1
Caelo	Flor de malva	13351301	2
Caelo	Flor de malva	13351303	2
Caelo	Flor de malva	9311104	1
Caelo	Flor de malva	13267301-3409310112	1
Caelo	Flor de malva	12187501-3414310132	1
Caesar & Loretz Gm...	Flor de malva	12187402	8
Caesar & Loretz Gm...	Flor de malva	13267301	6
Galke	Flor de malva	21119	1
Gehe	Flor de malva	1501B110207	1
Gehe	Flor de malva	1501B120508	6
Klenk	Flor de malva	10357908	2
Caelo	Flor de malva	12187505	3
Klenk	Flor de malva	1910211464	1
Klenk	Flor de malva	1501B120427	10
Klenk	Flor de malva	1501B111215	1
Klenk	Flor de malva	1501B-120427	1
Klenk	Flor de malva	B120427	1
Klenk	Flor de malva	B130829	3
Klenk	Flor de malva	1501b111215	1
Klenk	Flor de malva	1501B130829	3
Klenk	Flor de malva	150B111215	1
Klenk	Flor de malva	1501B100408	1
Nachprüfung 29.10.12	Flor de malva	C1316	1
Klenk	Flor de malva	1501b110207	1
Aurica / 11	Flor de prímula	521301234	1
Aurica/Gehe	Flor de prímula	521203308	1
Caelo	Flor de prímula	11206810	5
Caelo	Flor de prímula	11206808	1
Caelo	Flor de prímula	5021303	1
Caelo	Flor de prímula	9021301	1
Caelo	Flor de prímula	11206811	1
Caelo	Flor de prímula	11374403	1
Caelo	Flor de prímula	25091306	1
Caelo	Flor de prímula	11206807	1
Caelo	Flor de prímula	1308660	1
Caelo	Flor de prímula	13086608	1
Caelo	Flor de prímula	13276904	1
Caelo	Flor de prímula	13086603	5
Caelo	Flor de prímula	11374404	1
Caelo	Flor de prímula	113744044	1
Caelo	Flor de prímula	11374402	1
Caelo	Flor de prímula	11374401	10
Caelo	Flor de prímula	13086603	1
Caelo	Flor de prímula	13086602	5
Caelo	Flor de prímula	10207104	1
Caelo	Flor de prímula	11206803	4
Caelo	Flor de prímula	11206804	1
Caelo	Flor de prímula	10072509	1
Galke	Flor de prímula	22612	2
Gehe	Flor de prímula	11374401	1
Caelo	Flor de prímula	13086605	1
Klenk	Flor de prímula	1541B100414	1
Klenk	Flor de prímula	B110314	1
Klenk	Flor de prímula	B130808	1
Klenk	Flor de prímula	A111018	1
Klenk	Flor de prímula	B130808	1
Klenk	Flor de prímula	1540A-100907	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Flor de prímula	1540A100907	1
Klenk	Flor de prímula	1541B110314	7
Caelo	Flor de prímula	11206811	4
Caelo	Flor de prímula	11374403	3
Sanacorp	Flor de prímula	1541B130808	6
Caelo	Flor de prímula	13086602	3
VDL	Flor de prímula	11206806	1
Weltecke / GEHE	Flor de prímula	63011112	1
Caelo	Flor de rosa vermelha	12380008	2
Galke	Flor de rosa vermelha	22641	2
Klenk	Flor de rosa vermelha	1561A121016	1
Caelo	Flor de rosa vermelha	12380004	1
Caelo	Flor de tília	11086305	7
Bahnhof-Apotheke	Flor de tília	7-121011	1
Bombastus	Flor de tília	275129	2
Bombastus	Flor de tília	280678	3
Caelo	Flor de tília	9206604	1
Caelo	Flor de tília	10273608	2
Caelo	Flor de tília	11086307	3
Caelo	Flor de tília	272958	7
Caelo	Flor de tília	12170703	1
Caelo	Flor de tília	1210702	1
Caelo	Flor de tília	10273606	1
Caelo	Flor de tília	12170702	2
Caelo	Flor de tília	28031302	1
Caelo	Flor de tília	Int.Ch:210140	1
Caelo	Flor de tília	12170701	1
Caelo	Flor de tília	15111301	1
Caelo	Flor de tília	13337403	5
Caelo	Flor de tília	13101708	1
Caelo	Flor de tília	15068302	1
Caelo	Flor de tília	268709	2
Caelo	Flor de tília	13101701	7
Caelo	Flor de tília	12170702-3355319071	1
Caelo	Flor de tília	13337403-348012102	1
Caelo	Flor de tília	13101702	8
galke,	Flor de tília	2098	1
Klenk	Flor de tília	1611B120827	11
Klenk	Flor de tília	1611B130905	5
Klenk	Flor de tília	1611B110421	2
Klenk	Flor de tília	Pr.Nr.4411A-01474	1
Klenk	Flor de tília	B130307	2
Klenk	Flor de tília	1611B1010004	1
Klenk	Flor de tília	B130905	4
Klenk	Flor de tília	1611B131220	1
Klenk	Flor de tília	1611B121105	4
Klenk	Flor de tília	1611a121120	2
Klenk	Flor de tília	1611A121120	7
Klenk	Flor de tília	1611B111011	6
Klenk	Flor de tília	1611B130307	4
Phönix	Flor de tília	2090413	1
Phönix	Flor de tília	1611A12120	1
Sanacorp	Flor de tília	264045	1
Wolf	Flor de tília	B449	1
Wolf	Flor de tília	22094	1
Aurica	Flor de trevo vermelho	521206331	1
Aurica	Flor de trevo vermelho	521203442	1
Aurica/Anzag	Flor de trevo vermelho	521303918	1
Galke	Flor de trevo vermelho	23128	2
Klenk	Flor de trevo vermelho	7470A130311	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Flor de trevo vermelho	811Q-07163	1
Klenk	Flor de trevo vermelho	1640A110727	1
Klenk	Flor de trevo vermelho	1640a130122	1
Klenk	Flor de trevo vermelho	1640A130122	15
Kräuter Schulte	Flor de trevo vermelho	53778	1
Caelo	Flor de ulmária, separada	9326211	2
Caelo	Flor de ulmária, separada	9326213	2
Caelo	Flor de ulmária, separada	10349305	1
Caelo	Flor de ulmária, separada	1227501	1
Caelo	Flor de ulmária, separada	12275701	2
Caelo	Flor de ulmária, separada	10051301	1
Caelo	Flor de ulmária, separada	10349308	1
Caelo	Flor de ulmária, separada	1225702	1
Caelo	Flor de ulmária, separada	12275703	3
Caelo	Flor de ulmária, separada	12275704	4
Caelo	Flor de ulmária, separada	12275702	1
Caelo	Flor de ulmária, separada	10349302	2
Caelo	Flor de ulmária, separada	10349307	2
Caelo	Flor de ulmária, separada	12275704-3372319032	1
Klenk	Flor de ulmária, separada	A120312	1
Kräuter Schulte	Flor de ulmária, separada	51369	1
Kräuter Schulte	Flor de ulmária, separada	53473	1
Caelo	Flor de urtiga-branca	10081206	1
Caelo	Flor de urtiga-branca	12152402	2
Caelo	Flor de urtiga-branca	11371610	5
Caelo	Flor de urtiga-branca	11371609	3
Caelo	Flor de urtiga-branca	2101301	1
Caelo	Flor de urtiga-branca	11371613	2
Caelo	Flor de urtiga-branca	15299101	1
Caelo	Flor de urtiga-branca	52470437	1
Galke	Flor de urtiga-branca	21691	4
Galke	Flor de urtiga-branca	22704	1
Klenk	Flor de urtiga-branca	1470A120111	4
Caelo	Flor de urtiga-branca	11371611	2
Caelo	Flor de urtiga-branca	12275802	1
Klenk	Flor de urtiga-branca	1470A080103	1
Caelo	Flor de urze, separada	10270516	1
Caelo	Flor de urze, separada	13014204	5
Caelo	Flor de urze, separada	13014206	1
Klenk	Flor de urze, separada	13014202	1
Caelo	Flor de verbasco, cortada	12317104	1
Caelo	Flor de verbasco, cortada	521505390	1
Caelo	Flor de verbasco, cortada	11020802	2
Caelo	Flor de verbasco, cortada	11020902	1
Caelo	Flor de verbasco, cortada	16081201	1
Caelo	Flor de verbasco, cortada	11020714	4
Caelo	Flor de verbasco, cortada	11233401	4
Caelo	Flor de verbasco, cortada	11366402	1
Caelo	Flor de verbasco, cortada	12192901	3
Caelo	Flor de verbasco, cortada	12192903	3
Caelo	Flor de verbasco, cortada	18031301	1
Caelo	Flor de verbasco, cortada	11233402	1
Caelo	Flor de verbasco, cortada	11333402	1
Caelo	Flor de verbasco, cortada	12170901	1
Caelo	Flor de verbasco, cortada	12192904	1
Caelo	Flor de verbasco, cortada	12192907	3
Caelo	Flor de verbasco, cortada	13229702	1
Caelo	Flor de verbasco, cortada	11020713	2
Caelo	Flor de verbasco, cortada	1219203	1
Caelo	Flor de verbasco, cortada	12192905	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Flor de verbasco, cortada	11366403	1
Caelo	Flor de verbasco, cortada	12170906	1
Caelo	Flor de verbasco, cortada	13229701	2
Caesar/Noweda	Flor de verbasco, cortada	2810E-01475	1
Hepart AG	Flor de verbasco, cortada	12170904	2
Klenk	Flor de verbasco, cortada	1650A100608	1
Klenk	Flor de verbasco, cortada	1651B110203	2
Klenk	Flor de verbasco, cortada	1650A111018	3
Klenk	Flor de verbasco, cortada	A120612	1
Klenk	Flor de verbasco, cortada	1650A120612	1
Klenk	Flor de verbasco, cortada	1651B140324	2
Klenk	Flor de verbasco, cortada	1651B150722	1
Klenk	Flor de verbasco, cortada	1651B130820	5
Klenk	Flor de verbasco, cortada	1651b130820	2
Klenk	Flor de verbasco, cortada	1651B121109	22
Klenk	Flor de verbasco, cortada	1651B120315	3
Caelo	Flor de vulnerária, grossei…	13104301	2
Akazie	Folha de alecrim	20.09.2015	1
Bahnhof-Apotheke	Folha de alecrim	7-120915	1
Bomastus-Werke/Phönix	Folha de alecrim	298424	2
Bombastus	Folha de alecrim	277128	1
Bombastus	Folha de alecrim	293920	1
Bombastus	Folha de alecrim	281248	1
Bombastus	Folha de alecrim	287805	1
Bombastus	Folha de alecrim	270171	1
Bombastus	Folha de alecrim	281843	1
Caelo	Folha de alecrim	11193402	2
Caelo	Folha de alecrim	11193405	1
Caelo	Folha de alecrim	11193404	1
Caelo	Folha de alecrim	11193408	6
Caelo	Folha de alecrim	5041302	1
Caelo	Folha de alecrim	IntCh:313060	1
Caelo	Folha de alecrim	12225902	1
Caelo	Folha de alecrim	13128801	1
Caelo	Folha de alecrim	13128802	2
Caelo	Folha de alecrim	13128806	2
Caelo	Folha de alecrim	13128805	1
Caelo	Folha de alecrim	28051404	1
Caelo	Folha de alecrim	14082901	1
Caelo	Folha de alecrim	14159601	1
Caelo	Folha de alecrim	1415901	1
Caelo	Folha de alecrim	2261A7020901	1
Caelo	Folha de alecrim	17352502	1
Caelo	Folha de alecrim	11193406	1
Caelo	Folha de alecrim	11193405	1
Caelo	Folha de alecrim	15125001	2
Caelo	Folha de alecrim	15125008	1
Caelo	Folha de alecrim	15428003	1
Galke	Folha de alecrim	21390	1
Galke	Folha de alecrim	19813	1
Galke	Folha de alecrim	22777	1
Klenk	Folha de alecrim	301401	1
Klenk	Folha de alecrim	2261A120224	18
Klenk	Folha de alecrim	A130201	2
Klenk	Folha de alecrim		1
Klenk	Folha de alecrim	61A131118	1
Klenk	Folha de alecrim	2261A170803	1
Klenk	Folha de alecrim	2261A140910	4
Klenk	Folha de alecrim	2216A170803	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Folha de alecrim	2261A130201	29
Klenk	Folha de alecrim	2261A160329	2
Klenk	Folha de alecrim	112E-01510	1
Klenk	Folha de alecrim	2261A160905	6
Klenk	Folha de alecrim	2261A150622	6
Klenk	Folha de alecrim	2261A081117	1
Klenk	Folha de alecrim	2261a160329	1
Klenk	Folha de alecrim	2261A131118	13
Noweda	Folha de alecrim	2261A100916	1
Noweda	Folha de alecrim	15428011	1
Klenk	Folha de alecrim	2261a120224	2
Klenk	Folha de alecrim	2261A170317	1
Anzag	Folha de amora	10136412	1
Anzag 27.12.12 ek:2,79	Folha de amora	10136048	1
Bahnhof-Apotheke	Folha de amora	18-120702	1
Bombastus	Folha de amora	267122	1
Bombastus	Folha de amora	273668	2
Caelo	Folha de amora	2271c120508	1
Caelo	Folha de amora	10136403	1
Caelo	Folha de amora	10136408	6
Caelo	Folha de amora	28061202	1
Caelo	Folha de amora	13091206	1
Caelo	Folha de amora	11030704	4
Caelo	Folha de amora	11030707	5
Caelo	Folha de amora	3011E-01512	1
Caelo	Folha de amora	11030706	1
Caelo	Folha de amora	3091303	1
Caelo	Folha de amora	14111318	1
Caelo	Folha de amora	13127901	1
Caelo	Folha de amora	13101610	1
Caelo	Folha de amora	14019010	1
Caelo	Folha de amora	15039301	1
Caelo	Folha de amora	11030701	2
Gehe	Folha de amora	10136409	1
Klenk	Folha de amora	2271B111216	1
Caelo	Folha de arando vermelho, c...	12105201	1
Caelo	Folha de arando vermelho, c...	12105203	1
Caelo	Folha de arando vermelho, c...	12150205	1
Caelo	Folha de arando vermelho, c...	11334302	1
Klenk	Folha de arando vermelho, c...	2431B101006	2
Aurica	Folha de bétula	521205644	1
Bahnhof-Apotheke	Folha de bétula	18-120702	1
Bombastus	Folha de bétula	280677	1
Bombastus	Folha de bétula	287280	1
Bombastus	Folha de bétula	272385	1
Bombastus	Folha de bétula	267077	1
Bombastus	Folha de bétula	270743	1
Caelo	Folha de bétula	11189510	3
Caelo	Folha de bétula	11189507	1
Caelo	Folha de bétula	11189508	1
Caelo	Folha de bétula	12193109	15
Caelo	Folha de bétula	IntCh:311092	1
Caelo	Folha de bétula	12193108	1
Caelo	Folha de bétula	13108906	1
Caelo	Folha de bétula	13337303	1
Caelo	Folha de bétula	13337302	1
Caelo	Folha de bétula	13108917	1
Caelo	Folha de bétula	14360702	1
Caelo	Folha de bétula	13108916	1
Caelo	Folha de bétula	12193104	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de bétula	107063	1
Caelo	Folha de bétula	11189502	1
Caelo	Folha de bétula	12193004	5
Caelo	Folha de bétula	12193105	3
Caelo	Folha de bétula	13337303-3561412013	1
Caesar & Loretz Gm...	Folha de bétula	11050102	3
Fagron	Folha de bétula	7061301	1
Galke	Folha de bétula	20904	1
Galke	Folha de bétula	21226	1
Klenk	Folha de bétula	1901A110726	24
Klenk	Folha de bétula	1901c120508	1
Klenk	Folha de bétula	20111201	1
Klenk	Folha de bétula	1901C120508	18
Klenk	Folha de bétula	F-040413-1	1
Klenk	Folha de bétula	C120802	1
Klenk	Folha de bétula	21061303	1
Klenk	Folha de bétula	A121130	2
Klenk	Folha de bétula	1901A121130	24
Klenk	Folha de bétula	1901c120802	1
Klenk	Folha de bétula	28101306	1
Klenk	Folha de bétula	27121301	1
Klenk	Folha de bétula	1901A130218	5
Klenk	Folha de bétula	4021409	1
Klenk	Folha de bétula	1901A130318	2
Klenk	Folha de bétula	1901A140214	1
Klenk	Folha de bétula	1901A-110726	3
Klenk	Folha de bétula	1901C120802	19
Klenk	Folha de bétula	4213I01481	1
Klenk	Folha de bétula	1901A05051801	1
Klenk	Folha de bétula	4113A-01481	1
Caelo	Folha de bétula	13108905	8
Spangropharm	Folha de bétula	264603	1
Caelo	Folha de boldo	11016509	1
Caelo	Folha de boldo	655456	1
Caelo	Folha de boldo	11016511	1
Caelo	Folha de boldo	12064303	1
Caelo	Folha de boldo	12227005	1
Caelo	Folha de boldo	12064305	1
Caelo	Folha de boldo	12064306	1
Caelo	Folha de boldo	12227004	1
Galke	Folha de boldo	19855	1
Klenk	Folha de boldo	1911B090709	1
Klenk	Folha de boldo	1911A100714	7
VDL	Folha de boldo	11016503	1
Caelo	Folha de buchu	13056601	2
Caelo	Folha de buchu	13056602	2
Caelo	Folha de buchu	13056605	1
Kräuter Schulte	Folha de buchu	54519	1
Caelo	Folha de cardo aquático, cortada	12226101	1
Caelo	Folha de cardo aquático, cortada	1226101	1
Caelo	Folha de cardo aquático, cortada	13123901	2
Caelo	Folha de cardo aquático, cortada	13123902	2
Caelo	Folha de cardo aquático, cortada	12226104	1
Caesar/Noweda	Folha de cardo aquático, cortada	1510U-01517	1
Caelo	Folha de cardo aquático, cortada	13149001	1
Klenk	Folha de Damiana, cortada	12064101	1
Caelo	Folha de Damiana, cortada	12330402	7
Caelo	Folha de Damiana, cortada	12330403	2
Caelo	Folha de Damiana, cortada	12330401	5
Caelo	Folha de Damiana, cortada	12064103	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de Damiana, cortada	11026607	2
Caelo	Folha de Damiana, cortada	12330407	2
Klenk	Folha de Damiana, cortada	A130206	2
Klenk	Folha de Damiana, cortada	1990A130206	1
Noweda	Folha de Damiana, cortada	200151	1
Redwood	Folha de Damiana, cortada	216451	1
-	Folha de erva-cidreira	131146	1
Alfred Galke	Folha de erva-cidreira	D-NI-1-9516-BC	1
Bahnhof-Apotheke	Folha de erva-cidreira	17-120917	1
Bombastus	Folha de erva-cidreira	270044	1
Bombastus	Folha de erva-cidreira	271499	2
Bombastus	Folha de erva-cidreira	277722	1
Caelo	Folha de erva-cidreira		1
Caelo	Folha de erva-cidreira	1009	1
Caelo	Folha de erva-cidreira	CH.111111	1
Caelo	Folha de erva-cidreira	12032303	1
Caelo	Folha de erva-cidreira	12032309	1
Caelo	Folha de erva-cidreira	12032307	2
Caelo	Folha de erva-cidreira	12032316	3
Caelo	Folha de erva-cidreira	12032312	1
Caelo	Folha de erva-cidreira	25021301	1
Caelo	Folha de erva-cidreira	12032319	5
Caelo	Folha de erva-cidreira	19041303	1
Caelo	Folha de erva-cidreira	25061303	1
Caelo	Folha de erva-cidreira	13030805	1
Caelo	Folha de erva-cidreira	14111319	1
Caelo	Folha de erva-cidreira	24011407	1
Caelo	Folha de erva-cidreira	13214705	1
Caelo	Folha de erva-cidreira	13214720	1
Caelo	Folha de erva-cidreira	10310919	1
Caelo	Folha de erva-cidreira	12032318	1
Caelo	Folha de erva-cidreira	13030803	2
Caelo	Folha de erva-cidreira	2161a121009	1
galke	Folha de erva-cidreira	20867	1
Gehe	Folha de erva-cidreira	12032314	4
Klenk	Folha de erva-cidreira	2161A121206	2
Klenk	Folha de erva-cidreira	2161A151209	1
Klenk	Folha de erva-cidreira	111207	1
Klenk	Folha de erva-cidreira	2807211503	1
Klenk	Folha de erva-cidreira	2161A111207	15
Klenk	Folha de erva-cidreira	2161A110818	1
Klenk	Folha de erva-cidreira	27091201	1
Klenk	Folha de erva-cidreira	2161A120718	11
Klenk	Folha de erva-cidreira	2161A121009	14
Klenk	Folha de erva-cidreira	2161A121009/PN:1198	1
Klenk	Folha de erva-cidreira	2161A121029	4
Klenk	Folha de erva-cidreira	2161A101216	1
Caelo	Folha de erva-cidreira	13214707	1
Caelo	Folha de erva-cidreira	12032310	1
an	Folha de espinheiro-branco …	1971A130930	2
Bahnhof-Apotheke	Folha de espinheiro-branco …	7-121011	1
Bombastus	Folha de espinheiro-branco …	264044	1
Bombastus	Folha de espinheiro-branco …	267551	1
Bombastus	Folha de espinheiro-branco …	272881	1
Bombastus	Folha de espinheiro-branco …	267000	1
Bombastus	Folha de espinheiro-branco …	273287	1
Bombastus	Folha de espinheiro-branco …	278756	1
Caelo	Folha de espinheiro-branco …	10273512	2
Caelo	Folha de espinheiro-branco …	10273515	6
Caelo	Folha de espinheiro-branco …	11366001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de espinheiro-branco …	11068206	1
Caelo	Folha de espinheiro-branco …	12225104	12
Caelo	Folha de espinheiro-branco …	1222514	1
Caelo	Folha de espinheiro-branco …	12225108	7
Caelo	Folha de espinheiro-branco …	IntCh:313082	1
Caelo	Folha de espinheiro-branco …	12225107	5
Caelo	Folha de espinheiro-branco …	13276703	3
Caelo	Folha de espinheiro-branco …	15188802	1
Caelo	Folha de espinheiro-branco …	1518802	1
Caelo	Folha de espinheiro-branco …	16025802	1
Caelo	Folha de espinheiro-branco …	2225104	1
Caelo	Folha de espinheiro-branco …	109076	1
Caelo	Folha de espinheiro-branco …	1225107	1
Caelo	Folha de espinheiro-branco …	12225207	1
Caelo	Folha de espinheiro-branco …	52467476	1
Caelo	Folha de espinheiro-branco …	1221707	1
Galke	Folha de espinheiro-branco …	21126	3
Gehe	Folha de espinheiro-branco …	1351B111207	2
Kenk / Phoenix	Folha de espinheiro-branco …	1971A130307	6
Klenk	Folha de espinheiro-branco …	1971A110620	5
Klenk	Folha de espinheiro-branco …	1971A120215	3
Klenk	Folha de espinheiro-branco …	14101301	1
Klenk	Folha de espinheiro-branco …	28101307	1
Klenk	Folha de espinheiro-branco …	20121302	1
Klenk	Folha de espinheiro-branco …	A130307	1
Klenk	Folha de espinheiro-branco …	1971a120813	2
Klenk	Folha de espinheiro-branco …	1972A120727	1
Klenk	Folha de espinheiro-branco …	1971A120813	20
Klenk	Folha de espinheiro-branco …	1971A120727	13
Klenk	Folha de espinheiro-branco …	1971a120215	1
Klenk	Folha de espinheiro-branco …	1971A120813-34103101	1
Klenk	Folha de espinheiro-branco …	1971A130307-3447	1
Klenk	Folha de espinheiro-branco …	1971A130307-35014110	1
Bombastus	Folha de espinheiro-branco …	275310	2
vedono	Folha de espinheiro-branco …	12225103	4
Caelo	Folha de eucalipto	12225203	3
Klenk	Folha de eucalipto	2011B120419	6
Caelo	Folha de eucalipto	9346811	1
Caelo	Folha de eucalipto	12225202	1
Caelo	Folha de eucalipto	122250204	1
Caelo	Folha de eucalipto	12225206	1
Caelo	Folha de eucalipto	11307708	2
Klenk	Folha de eucalipto	B120419	1
Klenk	Folha de eucalipto	B130306	2
Klenk	Folha de eucalipto	2011B130306	4
Klenk	Folha de eucalipto	2011b130306	1
Klenk	Folha de eucalipto	2011B130306-35294110	1
VDL	Folha de eucalipto	2011B110801	4
-	Folha de framboesa	130849	1
AHD	Folha de framboesa	300696	1
Alfred Galke	Folha de framboesa	19851	1
an	Folha de framboesa	13086708	1
Anzag	Folha de framboesa	2291A120806	2
Anzag	Folha de framboesa	12103107	11
Anzag ek:3,00EUR 11.09.12	Folha de framboesa	12103105	18
Caelo	Folha de framboesa	1236705	1
Caelo	Folha de framboesa	10136412	1
Klenk	Folha de framboesa	2291A120507	5
Bahnhof-Apotheke	Folha de framboesa	17-120917	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Folha de framboesa	274507	1
Bombastus	Folha de framboesa	279686	3
Bombastus	Folha de framboesa	273668	2
Bombastus	Folha de framboesa	269870	1
Bombastus	Folha de framboesa	291500	1
Bombastus	Folha de framboesa	273778	1
Bombastus	Folha de framboesa	272898	1
Bombastus	Folha de framboesa	248586	1
Bombastus	Folha de framboesa	267122	1
Caelo	Folha de framboesa	1310603	1
Caelo	Folha de framboesa	10013407	1
Caelo	Folha de framboesa	307211511	1
Caelo	Folha de framboesa	10013411	1
Caelo	Folha de framboesa	9081205	1
Caelo	Folha de framboesa	22081201	1
Caelo	Folha de framboesa	25091201	1
Caelo	Folha de framboesa	2909211511	1
Caelo	Folha de framboesa	9101204	1
Caelo	Folha de framboesa	18101203	1
Caelo	Folha de framboesa	12103108	8
Caelo	Folha de framboesa	11121201	1
Caelo	Folha de framboesa	12103109	2
Caelo	Folha de framboesa	17121203	1
Caelo	Folha de framboesa	1210315	1
Caelo	Folha de framboesa	12362702	7
Caelo	Folha de framboesa	8031307	1
Caelo	Folha de framboesa	10013410	1
Caelo	Folha de framboesa	18041304	1
Caelo	Folha de framboesa	12362706	29
Caelo	Folha de framboesa	11030706	3
Caelo	Folha de framboesa	21051302	1
Caelo	Folha de framboesa	IntCh:311090	1
Caelo	Folha de framboesa	11071301	1
Caelo	Folha de framboesa	20081311	1
Caelo	Folha de framboesa	12362707	5
Caelo	Folha de framboesa	13038002	1
Caelo	Folha de framboesa	13038003	1
Caelo	Folha de framboesa	13101803	1
Caelo	Folha de framboesa	12362711	9
Caelo	Folha de framboesa	12362708	4
Caelo	Folha de framboesa	10136408	1
Caelo	Folha de framboesa	7011402	1
Caelo	Folha de framboesa	9011404	1
Caelo	Folha de framboesa	13127901	3
Caelo	Folha de framboesa	30011408	1
Caelo	Folha de framboesa	14018803	1
Caelo	Folha de framboesa	12103101	7
Caelo	Folha de framboesa	2271C120508	5
Caelo	Folha de framboesa	12362704	5
Caelo	Folha de framboesa	713E-01511	1
Caelo	Folha de framboesa	11030707	4
Caelo	Folha de framboesa	12362705	9
Caelo	Folha de framboesa	314U1511	1
Caelo	Folha de framboesa	12392709	1
Caelo	Folha de framboesa	6859427	1
Caelo	Folha de framboesa	12368706	1
Caelo	Folha de framboesa	12362709	7
Caelo	Folha de framboesa	231013c	1
Caelo	Folha de framboesa	10136404	1
Caelo	Folha de framboesa	12362710	14

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de framboesa	12362710-3432311160	1
Caelo	Folha de framboesa	13101604	3
Caelo	Folha de framboesa	13101602-347312141	1
Caesar & Loretz Gm…	Folha de framboesa	10013408	1
China Medica	Folha de framboesa	13086703	1
Galke	Folha de framboesa	21244	1
Galke	Folha de framboesa	18060	2
Galke	Folha de framboesa	19499	2
Galke	Folha de framboesa	23532	1
gehe 10.12.13	Folha de framboesa	229117121120	1
Gutenberg-Apotheke	Folha de framboesa	28911	1
Klenk	Folha de framboesa	2291A12112o	1
Caelo	Folha de framboesa	11030705	1
Caelo	Folha de framboesa	13101605	1
Kenk / Phoenix	Folha de framboesa	22781C120508	1
Klenk	Folha de framboesa	2291A-120806	1
Klenk	Folha de framboesa	12273107	1
Klenk	Folha de framboesa	2291A130320	1
Klenk	Folha de framboesa	A130430	1
Klenk	Folha de framboesa	2291A121120	4
Klenk	Folha de framboesa	2291A120813	2
Klenk	Folha de framboesa	2291a111124	1
Klenk	Folha de framboesa	2291A110125	1
Phoenix	Folha de framboesa	10136409	1
Caelo	Folha de framboesa	12130107	1
Phönix	Folha de framboesa	12362701	7
Caelo	Folha de framboesa	12103111	15
Klenk	Folha de framboesa	2291A111124	1
Sanacorp	Folha de framboesa	12362703	9
Sanacorp	Folha de framboesa	13038001	6
Caelo	Folha de framboesa	10013409	2
Caelo	Folha de framboesa	13101603	6
Caelo	Folha de framboesa	11030704	2
VDL	Folha de framboesa	10013406	3
Wolf	Folha de framboesa	P201727	19
Wolf	Folha de framboesa	P222676	1
Wolf	Folha de framboesa	B-457	1
Caelo	Folha de freixo, cortada	12225504	1
Caelo	Folha de freixo, cortada	12225502	1
Caelo	Folha de freixo, cortada	12225505	2
Klenk	Folha de freixo, cortada	5111A-01491	1
Caelo	Folha de ginkgo	12151709	2
Caelo	Folha de ginkgo	15077407	1
Caelo	Folha de ginkgo	13340907	1
Caelo	Folha de ginkgo	13340904	1
Caelo	Folha de ginkgo	13340906	1
Caelo	Folha de ginkgo	12373604	1
Caelo	Folha de ginkgo	15077410	1
Nachprüfung	Folha de ginkgo	2461A100429	11
Caelo	Folha de groselha, cortada	9373913	1
Caelo	Folha de groselha, cortada	12115902	1
Caelo	Folha de groselha, cortada	12168804	1
Caelo	Folha de groselha, cortada	12168810	3
Caelo	Folha de groselha, cortada	80558228	1
Klenk	Folha de groselha, cortada	2251a110204	1
Nachprüfung	Folha de groselha, cortada	1003	1
Sanacorp	Folha de groselha, cortada	2251A110204	4
Caelo	Folha de hamamélis	10102915	1
Caelo	Folha de hamamélis	12165805	1
Caelo	Folha de hamamélis	12164802	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de hamamélis	14356103	1
Caelo	Folha de hamamélis	30287394	1
Caelo	Folha de hamamélis	13269904	1
Caelo	Folha de hamamélis	13269902	2
Caelo	Folha de hamamélis	12164804	1
Euro OTC	Folha de hamamélis	12164805	1
Klenk	Folha de hamamélis	B110214	1
Klenk	Folha de hamamélis	2051B110214	1
Caelo	Folha de hamamélis	13269905	1
Caelo	Folha de hera, cortada	23121303	1
Caelo	Folha de hera, cortada	23121305	1
Caelo	Folha de hera, cortada	8061205	1
Caelo	Folha de hera, cortada	11101205	1
Caelo	Folha de hera, cortada	15101203	1
Caelo	Folha de hera, cortada	20111211	1
Caelo	Folha de hera, cortada	4011301	1
Caelo	Folha de hera, cortada	11229505	5
Caelo	Folha de hera, cortada	2031301	1
Caelo	Folha de hera, cortada	12225603	2
Caelo	Folha de hera, cortada	11041303	1
Caelo	Folha de hera, cortada	12225602	1
Caelo	Folha de hera, cortada	27111301	1
Caelo	Folha de hera, cortada	10011401	1
Caesar & Loretz/ Noweda	Folha de hera, cortada	12225606	5
Gehe	Folha de hera, cortada	2061B080402	1
Klenk	Folha de hera, cortada	B130118	1
Phönix	Folha de hera, cortada	11101102	1
Caelo	Folha de hera, cortada	12225605	5
Bombastus	Folha de hortelã-pimenta	266772	2
Bombastus	Folha de hortelã-pimenta	275295	3
Bombastus	Folha de hortelã-pimenta	246514	1
Bombastus	Folha de hortelã-pimenta	272956	3
Bombastus	Folha de hortelã-pimenta	279634	1
Bombastus	Folha de hortelã-pimenta	279214	1
Bombastus	Folha de hortelã-pimenta	281282	1
Bombastus	Folha de hortelã-pimenta	281043	3
Bombastus	Folha de hortelã-pimenta	271499	1
Bombastus	Folha de hortelã-pimenta	285914	1
Bombastus	Folha de hortelã-pimenta	276514	1
Bombastus	Folha de hortelã-pimenta	278679	2
Bombastus	Folha de hortelã-pimenta	286105	1
Bombastus	Folha de hortelã-pimenta	279914	2
Bombastus	Folha de hortelã-pimenta	255719	1
Bombastus	Folha de hortelã-pimenta	282509	1
Caelo	Folha de hortelã-pimenta	20061202	1
Caelo	Folha de hortelã-pimenta	11327803	5
Caelo	Folha de hortelã-pimenta	20111215	1
Caelo	Folha de hortelã-pimenta	11294409	2
Caelo	Folha de hortelã-pimenta	11327801	2
Caelo	Folha de hortelã-pimenta	11327808	3
Caelo	Folha de hortelã-pimenta	1132803	1
Caelo	Folha de hortelã-pimenta	12266903	5
Caelo	Folha de hortelã-pimenta	12266908	8
Caelo	Folha de hortelã-pimenta	2181B090928	1
Caelo	Folha de hortelã-pimenta	13030805	5
Caelo	Folha de hortelã-pimenta	Int.Ch.:313011	1
Caelo	Folha de hortelã-pimenta	ChB:311092	1
Caelo	Folha de hortelã-pimenta	13030806	1
Caelo	Folha de hortelã-pimenta	5091307	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de hortelã-pimenta	13030809	2
Caelo	Folha de hortelã-pimenta	13030808	1
Caelo	Folha de hortelã-pimenta	8101301	1
Caelo	Folha de hortelã-pimenta	12032311	1
Caelo	Folha de hortelã-pimenta	13030804	1
Caelo	Folha de hortelã-pimenta	161212	1
Caelo	Folha de hortelã-pimenta	12266912	1
Caelo	Folha de hortelã-pimenta	13214706	1
Caelo	Folha de hortelã-pimenta	6011403	1
Caelo	Folha de hortelã-pimenta	13214720	1
Caelo	Folha de hortelã-pimenta	14083102	2
Caelo	Folha de hortelã-pimenta	14221701	1
Caelo	Folha de hortelã-pimenta	14339202	2
Caelo	Folha de hortelã-pimenta	13214707	3
Caelo	Folha de hortelã-pimenta	268320	1
Caelo	Folha de hortelã-pimenta	12054149	1
Caelo	Folha de hortelã-pimenta	13030807	3
Caelo	Folha de hortelã-pimenta	11294401	3
Caelo	Folha de hortelã-pimenta	13214705	1
Caelo	Folha de hortelã-pimenta	12266904	3
Caelo	Folha de hortelã-pimenta	11347609	1
Caelo	Folha de hortelã-pimenta	2181A1209-13	1
Caelo	Folha de hortelã-pimenta	12032319	2
Caelo	Folha de hortelã-pimenta	13105001	1
Caelo	Folha de hortelã-pimenta	17117806	1
Caelo	Folha de hortelã-pimenta	17292709	1
Caelo	Folha de hortelã-pimenta	18287701	1
Caelo	Folha de hortelã-pimenta	17292702	1
Caelo	Folha de hortelã-pimenta	13030808-3401310161	1
Caelo	Folha de hortelã-pimenta	12266908-343431160	1
Caesar & Loretz GmbH	Folha de hortelã-pimenta	11294411	1
Fagron	Folha de hortelã-pimenta	1234567	2
Fagron	Folha de hortelã-pimenta	13030803	3
Fiebig ek:9.84EUR 24…	Folha de hortelã-pimenta	2181A110512	5
Galke	Folha de hortelã-pimenta	22218	1
Galke	Folha de hortelã-pimenta	20975	3
Galke	Folha de hortelã-pimenta	22783	3
Gehe	Folha de hortelã-pimenta	2181B130717A	1
Gehe	Folha de hortelã-pimenta	2181B130717B	1
Caelo	Folha de hortelã-pimenta	12266913	9
Hepart AG	Folha de hortelã-pimenta	B-185	5
HiperScan	Folha de hortelã-pimenta		1
Klenk	Folha de hortelã-pimenta	1209211505	1
Klenk	Folha de hortelã-pimenta	2181A-101013	1
Klenk	Folha de hortelã-pimenta	1001311505	1
Klenk	Folha de hortelã-pimenta	2161A110207	1
Klenk	Folha de hortelã-pimenta	1913A-01505	1
Klenk	Folha de hortelã-pimenta	2161A121009	6
Klenk	Folha de hortelã-pimenta	2183A120913	2
Klenk	Folha de hortelã-pimenta	2161A120718	3
Klenk	Folha de hortelã-pimenta	2181A130320	6
Klenk	Folha de hortelã-pimenta	216A121029	1
Klenk	Folha de hortelã-pimenta	2161A121206	14
Klenk	Folha de hortelã-pimenta	2161	1
Klenk	Folha de hortelã-pimenta	A121009	1
Klenk	Folha de hortelã-pimenta	2161A111207	1
Klenk	Folha de hortelã-pimenta	A130806	1
Klenk	Folha de hortelã-pimenta	2181B130717	10
Klenk	Folha de hortelã-pimenta	CH.2161B080818	1
Klenk	Folha de hortelã-pimenta	2161A130806	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Folha de hortelã-pimenta	2181A13020	1
Klenk	Folha de hortelã-pimenta	2161B140321	1
Klenk	Folha de hortelã-pimenta	2181A151119	1
Klenk	Folha de hortelã-pimenta	2181a120913	3
Klenk	Folha de hortelã-pimenta	2181B180727	2
Klenk	Folha de hortelã-pimenta	2181A190508-06	1
Klenk	Folha de hortelã-pimenta	4513E1503	1
Klenk	Folha de hortelã-pimenta	2161A07020203	1
Klenk	Folha de hortelã-pimenta	2181A-120913	1
Klenk	Folha de hortelã-pimenta	2181A100323	1
Klenk	Folha de hortelã-pimenta	2181A120913	34
Klenk	Folha de hortelã-pimenta	4113Q1505	1
Klenk	Folha de hortelã-pimenta	2181A171025	1
Klenk	Folha de hortelã-pimenta	2181a171109	1
Klenk	Folha de hortelã-pimenta	2181A190508	2
Klenk	Folha de hortelã-pimenta	2161A121029	17
Klenk	Folha de hortelã-pimenta	2181A180130	2
Klenk	Folha de hortelã-pimenta	2161A-121206	1
Kräuter-Schulte	Folha de hortelã-pimenta	56254	1
nachprüfung	Folha de hortelã-pimenta	C1327	1
Noweda	Folha de hortelã-pimenta	2911U-01505	1
Bombastus	Folha de hortelã-pimenta	273843	2
Klenk	Folha de hortelã-pimenta	2181A101013	6
Probe	Folha de hortelã-pimenta	1223456	1
Wolf	Folha de hortelã-pimenta	P221379	7
Wolf	Folha de hortelã-pimenta	B-120	1
Wolf	Folha de hortelã-pimenta	B243	1
Wolf	Folha de hortelã-pimenta	B-725	2
Wolf	Folha de hortelã-pimenta	B725	1
Caelo	Folha de louro	12299106	3
Caelo	Folha de louro	12299101	1
Klenk	Folha de louro	B110809	1
Klenk	Folha de louro, cortada	B110809	2
Caelo	Folha de malva	28061203	1
Caelo	Folha de malva	2131B120529	3
Caelo	Folha de malva	12310001	3
Caelo	Folha de malva	12310004	4
Caelo	Folha de malva	12310009	2
Caelo	Folha de malva	12310008	1
Caelo	Folha de malva	20111302	1
Caelo	Folha de malva	14073902	1
Caelo	Folha de malva	13174213	1
Caelo	Folha de malva	12153403	1
Caelo	Folha de malva	10290515	1
Caelo	Folha de malva	10290502	1
Caelo	Folha de malva	13174207	1
Galke	Folha de malva	17133	1
Galke	Folha de malva	21454	1
Galke	Folha de malva	21445	1
Gehe	Folha de malva	2131B110420	2
Gehe	Folha de malva	10290512	1
Klenk	Folha de malva	2131B10529	1
Klenk	Folha de malva	2131B130225	4
Klenk	Folha de malva	B130225	1
Sanacorp	Folha de malva	278925	1
Caelo	Folha de malva	13174217	1
Caelo	Folha de malva	12310006	1
Caelo	Folha de marshmallow	12328202	3
Caelo	Folha de marshmallow	12328206	3
Caelo	Folha de marshmallow	13199604	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de marshmallow	12328207	2
Caelo	Folha de mate	12133803	3
Caelo	Folha de mate	2141A120821	2
Caelo	Folha de mate	13061202	1
Caelo	Folha de mate	12133806	1
Caelo	Folha de mate	13118003	4
Caelo	Folha de mate	12133801	3
Caelo	Folha de mate	11091710	1
Caelo	Folha de mate	12133804	7
Caelo	Folha de mate	13118001	1
Caelo	Folha de mate	12133807	7
Caesar & Loretz Gm...	Folha de mate	13118002	10
Galke	Folha de mate	22365	1
Klenk	Folha de mate	2141A111213	16
Klenk	Folha de mate	2131A111213	1
Klenk	Folha de mate	2141A-111213	1
Klenk	Folha de mate	2141a111213	1
Bombastus	Folha de mirtilo	272176	2
Caelo	Folha de mirtilo	13009904	3
Caelo	Folha de mirtilo	9367603	2
Caelo	Folha de mirtilo	23111201	1
Caelo	Folha de mirtilo	12140206	2
Caelo	Folha de mirtilo	3091302	1
Caelo	Folha de mirtilo	13009907	2
Caelo	Folha de mirtilo	12140201	2
Caelo	Folha de mirtilo	13009901	3
Caelo	Folha de mirtilo	13009903	4
Caelo	Folha de mirtilo	1300907	1
Klenk	Folha de mirtilo	4042013	1
Klenk	Folha de mirtilo	2191N110516	5
Klenk	Folha de mirtilo	N110516	1
Sanacorp	Folha de mirtilo	2191A130410	2
Caelo	Folha de mirtilo	12140204	4
Caelo	Folha de morango	11117909	1
Caelo	Folha de morango	5122013c	1
Klenk	Folha de morango	2031B110224	2
Klenk	Folha de morango	B120925	1
Klenk	Folha de morango	A130430	1
Klenk	Folha de morango	2031A130430	2
ANZAG	Folha de nogueira	12124603	15
Anzag ek: 4,58EUR 25...	Folha de nogueira	2111A120123	9
Caelo	Folha de nogueira	11103010	5
ApoFit/Noweda	Folha de nogueira	271137	1
Caelo	Folha de nogueira	10050416	1
Caelo	Folha de nogueira	11103003	2
Caelo	Folha de nogueira	11103004	2
Caelo	Folha de nogueira	11103007	6
Caelo	Folha de nogueira	11103008	5
Caelo	Folha de nogueira	3051301	1
Caelo	Folha de nogueira	1214603	1
Caelo	Folha de nogueira	11103001	1
Caelo	Folha de nogueira	12124602	3
Caelo	Folha de nogueira	25041404	1
Caelo	Folha de nogueira	12124502	1
Caelo	Folha de nogueira	14064903	1
Caelo	Folha de nogueira	14064906	3
Caelo	Folha de nogueira	8071502	1
Caelo	Folha de nogueira	15126004	1
Caelo	Folha de nogueira	15126003	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de nogueira	1005903	1
Caelo	Folha de nogueira	12124601	8
Caelo	Folha de nogueira	16044002	4
Caelo	Folha de nogueira	16044008	1
Caelo	Folha de nogueira	15126002	1
Caelo	Folha de nogueira	3712Q-01499	1
Caelo	Folha de nogueira	12124603-341930192	1
Caelo	Folha de nogueira	1414Q01499	1
Caelo	Folha de nogueira	14064909	2
Caelo	Folha de nogueira	14064910	1
Caelo	Folha de nogueira	14064902	5
Caelo	Folha de nogueira	4713U01499	1
Caelo	Folha de nogueira	414Q1499	1
Caelo	Folha de nogueira	12124605	8
Caelo	Folha de nogueira	14064904	4
Caelo	Folha de nogueira	15126008	6
Galke	Folha de nogueira	21061	1
Gehe	Folha de nogueira	10050412	1
Gehe	Folha de nogueira	2111B151028	3
Hepart AG	Folha de nogueira	A120123	1
Caelo	Folha de nogueira	11103009	1
Klenk	Folha de nogueira	2111A110816	1
Klenk	Folha de nogueira	F-280513-1	1
Klenk	Folha de nogueira	A130410	1
Klenk	Folha de nogueira	2111A131029	1
Klenk	Folha de nogueira	2111A130410	4
Klenk	Folha de nogueira	2111A-120123	1
Klenk	Folha de nogueira	211B151028	1
noweda	Folha de nogueira		1
Caelo	Folha de oliveira	12159805	1
Caelo	Folha de oliveira	15254406	1
Caelo	Folha de oliveira	18100501	1
Klenk	Folha de oliveira	2211B131025	1
Klenk	Folha de oliveira	2211B130425	3
Klenk	Folha de oliveira	2211B120417	2
Klenk	Folha de oliveira	2211B150818	1
Anzag ek: 3,06 11…	Folha de sálvia	2301A120403	38
Aurica	Folha de sálvia	521204613	1
Bahnhof-Apotheke	Folha de sálvia	3-121018	1
Bombastus	Folha de sálvia	270115	1
Bombastus	Folha de sálvia	271253	1
Bombastus	Folha de sálvia	277512	1
Bombastus	Folha de sálvia	255381	1
Caelo	Folha de sálvia	11056109	5
Caelo	Folha de sálvia	22061201	1
Caelo	Folha de sálvia	22081203	1
Caelo	Folha de sálvia	31081202	1
Caelo	Folha de sálvia	1209211513	1
Caelo	Folha de sálvia	11056123	5
Caelo	Folha de sálvia	410211513	1
Caelo	Folha de sálvia	111012004	1
Caelo	Folha de sálvia	11056125	3
Caelo	Folha de sálvia	11347508	3
Caelo	Folha de sálvia	12112101	1
Caelo	Folha de sálvia	22111203	1
Caelo	Folha de sálvia	15121201	1
Caelo	Folha de sálvia	20121201	1
Caelo	Folha de sálvia	11347511	9
Caelo	Folha de sálvia	11347509	4
Caelo	Folha de sálvia	12021302	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de sálvia	103311513	1
Caelo	Folha de sálvia	12370001	18
Caelo	Folha de sálvia	15041304	1
Caelo	Folha de sálvia	11347513	1
Caelo	Folha de sálvia	12370006	8
Caelo	Folha de sálvia	17061302	1
Caelo	Folha de sálvia	25061302	1
Caelo	Folha de sálvia	312010	1
Caelo	Folha de sálvia	26081301	1
Caelo	Folha de sálvia	12370004	2
Caelo	Folha de sálvia	14111315	1
Caelo	Folha de sálvia	9121302	1
Caelo	Folha de sálvia	12370015	2
Caelo	Folha de sálvia	8011420	1
Caelo	Folha de sálvia	13011405	1
Caelo	Folha de sálvia	12370017	1
Caelo	Folha de sálvia	13266603	2
Caelo	Folha de sálvia	13266605	3
Caelo	Folha de sálvia	13266606	1
Caelo	Folha de sálvia	13266621	1
Caelo	Folha de sálvia	13266626	1
Caelo	Folha de sálvia	12370013	3
Caelo	Folha de sálvia	279939	1
Caelo	Folha de sálvia	11347503	1
Caelo	Folha de sálvia	12380009	1
Caelo	Folha de sálvia	1237003	1
Caelo	Folha de sálvia	123770010	1
Caelo	Folha de sálvia	12370011	11
Caelo	Folha de sálvia	12370003-3359319071	1
Caelo	Folha de sálvia	12370014-3477312161	1
Caelo	Folha de sálvia	12370014	8
Caelo	Folha de sálvia	12370009	12
Caesar & Loretz Gm…	Folha de sálvia	11056121	3
Caesar & Loretz Gm…	Folha de sálvia	11347502	5
Caesar & Loretz Gm…	Folha de sálvia	12370002	4
Caesar & Loretz Gm…	Folha de sálvia	12370010	16
Caesar & Loretz Gm…	Folha de sálvia	12370016	9
Finze	Folha de sálvia	2301A110204	7
Galke	Folha de sálvia	21015	3
gehe 07.12.2013	Folha de sálvia	2301/7120403	1
Kenk / Phoenix	Folha de sálvia	2301A130904	2
Klenk	Folha de sálvia	C120126	1
Klenk	Folha de sálvia	2301A110420	1
Klenk	Folha de sálvia	2301C12126	1
Klenk	Folha de sálvia	2301a120403	1
Klenk	Folha de sálvia	2301c120126	1
Klenk	Folha de sálvia	2301C12026	1
Klenk	Folha de sálvia	2301C120126	16
Klenk	Folha de sálvia	2301A110420	2
Nachprüfung 21.11.11	Folha de sálvia	C1247	1
Phoenix	Folha de sálvia	231C130326	1
Caelo	Folha de sálvia	12370003	4
Wolf	Folha de sálvia	B735	1
Bomba/AHD	Folha de sene	280008	1
Bombastus	Folha de sene	280448	1
Bombastus	Folha de sene	273547	3
Bombastus	Folha de sene	278109	1
Bombastus	Folha de sene	273474	1
Bombastus	Folha de sene	280581	2
Caelo	Folha de sene	11277304	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de sene	806211514	1
Caelo	Folha de sene	11277305	1
Caelo	Folha de sene	11277316	4
Caelo	Folha de sene	18071201	1
Caelo	Folha de sene	2909211514	1
Caelo	Folha de sene	711211514	1
Caelo	Folha de sene	1273103	1
Caelo	Folha de sene	12273107	9
Caelo	Folha de sene	103311514	2
Caelo	Folha de sene	12273105	6
Caelo	Folha de sene	1803311514	1
Caelo	Folha de sene	11041009	1
Caelo	Folha de sene	12273114	2
Caelo	Folha de sene	2231B13014	1
Caelo	Folha de sene	2413Q01514	1
Caelo	Folha de sene	12273120	5
Caelo	Folha de sene	12115502	1
Caelo	Folha de sene	9071302	1
Caelo	Folha de sene	12276111	1
Caelo	Folha de sene	313082	1
Caelo	Folha de sene	5091306	1
Caelo	Folha de sene	13136703	3
Caelo	Folha de sene	1316703	2
Caelo	Folha de sene	15101303	1
Caelo	Folha de sene	111113a	1
Caelo	Folha de sene	21011401	1
Caelo	Folha de sene	12369903	1
Caelo	Folha de sene	14183805	2
Caelo	Folha de sene	14306310	1
Caelo	Folha de sene	14306311	2
Caelo	Folha de sene	14306324	1
Caelo	Folha de sene	12273106	3
Caelo	Folha de sene	12273115	11
Caelo	Folha de sene	10126502	1
Caelo	Folha de sene	12273111	10
Caelo	Folha de sene	19135513	3
Caelo	Folha de sene	19135519	2
Caelo	Folha de sene	191355003	1
Caelo	Folha de sene	12273118	3
Caelo	Folha de sene	3813E1514	1
Caelo	Folha de sene	4113Q1514	1
Caelo	Folha de sene	5013U01514	1
Caelo	Folha de sene	131316701	1
Caelo	Folha de sene	2331B120521	4
Caelo	Folha de sene	514R1514	1
Caelo	Folha de sene	18046104	2
Caelo	Folha de sene	18046209	1
Caelo	Folha de sene	12273104	2
Caelo	Folha de sene	18046110	1
Caelo	Folha de sene	19135501	1
Caelo	Folha de sene	12115503	6
Caelo	Folha de sene	12273113	3
Caelo	Folha de sene	12273119	4
Caelo	Folha de sene	13136704	13
Caelo	Folha de sene	13136705-3489312103	1
Caelo	Folha de sene	13136706	1
Caelo	Folha de sene	1316706	1
Caesar & Loretz Gm…	Folha de sene	11277303	3
Caesar & Loretz Gm…	Folha de sene	11277308	3
Caesar & Loretz Gm…	Folha de sene	11277314	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz Gm...	Folha de sene	12273103	11
Caesar & Loretz Gm...	Folha de sene	13136708	7
Caesar&Loretz GmbH...	Folha de sene	12115504	4
Cealo	Folha de sene	12273116	15
Fagron	Folha de sene	314Q1514	1
Galke	Folha de sene	21778	1
Caelo	Folha de sene	13136705	4
Klenk	Folha de sene	2331A100525	2
Klenk	Folha de sene	2331B120403	1
Klenk	Folha de sene	2331B150903	1
Klenk	Folha de sene	2331B110907	2
Klenk	Folha de sene	2331C120614	8
Klenk	Folha de sene	2331B130214	5
Klenk	Folha de sene	B130214	1
Klenk	Folha de sene	2331C130326	16
Klenk	Folha de sene	2331c130326	1
Klenk	Folha de sene	2331A110207	1
Caelo	Folha de sene	13136718	1
Caelo	Folha de sene	13136724	1
Phönix 10.01.2014	Folha de sene	13136707	1
Sanacorp	Folha de sene	13136701	6
Caelo	Folha de sene	11277307	1
Caelo	Folha de sene	11277301	1
Caelo	Folha de sene	12115501	5
Caelo	Folha de sene	12273101	4
Caelo	Folha de sene pulverizada	11193307	1
Caelo	Folha de sene pulverizada	15363922	1
Caelo	Folha de sene pulverizada	17223202	1
Caelo	Folha de sene pulverizada	14347606	1
Caleo/ Fiebig	Folha de sene pulverizada	15363902	1
Fiebig	Folha de sene pulverizada	15363920	1
Klenk	Folha de sene pulverizada	2331B150903	1
Caelo	Folha de tília, cortada	1611A121120	1
Klenk	Folha de tília, cortada	2471B120502	1
Anzag	Folha de urtiga	2381-A130122	1
Anzag EK4,31 17.08.12	Folha de urtiga	2381A110913	19
Klenk	Folha de urtiga	2381a120619	4
Bahnhof-Apotheke	Folha de urtiga	7-121109	1
Bombastus	Folha de urtiga	266638	1
Bombastus	Folha de urtiga	270987	3
Bombastus	Folha de urtiga	270854	3
Bombastus	Folha de urtiga	273229	2
Bombastus	Folha de urtiga	275848	3
Bombastus	Folha de urtiga	280305	2
Bombastus	Folha de urtiga	276407	2
Bombastus	Folha de urtiga	266099	1
Bombastus	Folha de urtiga	275763	1
Caelo	Folha de urtiga	12183908	5
Caelo	Folha de urtiga	10291405	2
Caelo	Folha de urtiga	10282807	2
Caelo	Folha de urtiga	10282806	1
Caelo	Folha de urtiga		3
Caelo	Folha de urtiga	18071202	1
Caelo	Folha de urtiga	10291413	1
Caelo	Folha de urtiga	120375901	1
Caelo	Folha de urtiga	10291411	2
Caelo	Folha de urtiga	12195101	3
Caelo	Folha de urtiga	17121205	1
Caelo	Folha de urtiga	12184503	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Folha de urtiga	10375901	2
Caelo	Folha de urtiga	12184702	2
Caelo	Folha de urtiga	7031302	1
Caelo	Folha de urtiga	12184706	3
Caelo	Folha de urtiga	12184001	6
Caelo	Folha de urtiga	2051302	1
Caelo	Folha de urtiga	12814001	1
Caelo	Folha de urtiga	29071303	1
Caelo	Folha de urtiga	intch:313011	1
Caelo	Folha de urtiga	12183901	2
Caelo	Folha de urtiga	1283910	1
Caelo	Folha de urtiga	13091302	1
Caelo	Folha de urtiga	12183911	16
Caelo	Folha de urtiga	12183909	1
Caelo	Folha de urtiga	20111306	1
Caelo	Folha de urtiga	3021401	1
Caelo	Folha de urtiga	12034414	1
Caelo	Folha de urtiga	13386801	1
Caelo	Folha de urtiga	14344907	1
Caelo	Folha de urtiga	10162712	1
Caelo	Folha de urtiga	10291414	3
Caelo	Folha de urtiga	12184502	2
Caelo	Folha de urtiga	12184004	9
Caelo	Folha de urtiga	12195002	2
Caelo	Folha de urtiga	12183910	11
Caelo	Folha de urtiga	10291422	3
Caelo	Folha de urtiga	2381A130122	27
Caelo	Folha de urtiga	72085497	1
Caelo	Folha de urtiga	83374109	1
Caelo	Folha de urtiga	83142389	1
Caelo	Folha de urtiga	17337321	2
Caelo	Folha de urtiga	12183908-3391311070	1
Caelo	Folha de urtiga	12183908-3405310181	1
Caelo	Folha de urtiga	12183908-3443311112	1
Caelo	Folha de urtiga	12034403	8
Caelo	Folha de urtiga	12034402	3
Caesar & Loretz Gm…	Folha de urtiga	10291423	6
Galke	Folha de urtiga	20956	1
Galke	Folha de urtiga	21238	1
Galke	Folha de urtiga	23302	1
Gehe	Folha de urtiga	10162701	1
Gehe	Folha de urtiga	2381A120619	14
Gutenberg-Apotheke	Folha de urtiga	18897	1
Hepart AG	Folha de urtiga	P234605kbA	1
Klenk	Folha de urtiga	2381A-120619	1
Klenk	Folha de urtiga	2381A150109	1
Klenk	Folha de urtiga	2381A151012	1
Klenk	Folha de urtiga	1107211689	1
Klenk	Folha de urtiga	1913A-03054	1
Klenk	Folha de urtiga	A110913	1
Klenk	Folha de urtiga	2381A130703	15
Klenk	Folha de urtiga	A130703	1
Klenk	Folha de urtiga	2381a130703	1
Klenk	Folha de urtiga	A130122	1
Klenk	Folha de urtiga	2372A130703	1
Klenk	Folha de urtiga	2381A140221	1
Klenk	Folha de urtiga	2381A141124	1
Klenk	Folha de urtiga	2381A121010	1
Klenk	Folha de urtiga	114Q-03054	1
Klenk	Folha de urtiga	4513E3054	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Folha de urtiga	2381a130122	1
Klenk	Folha de urtiga	2381A-121010	1
Klenk	Folha de urtiga	2381A110809	1
Nachprüfung 8.2.13	Folha de urtiga	C1081	1
Noweda	Folha de urtiga	12195001	7
Caelo	Folha de urtiga	12183914	9
Sanacorp	Folha de urtiga	12184707	11
Sanacorp	Folha de urtiga	12184003	17
Caelo	Folha de urtiga	12184005	7
Caelo	Folha de urtiga	33/AD1	1
Wolf	Folha de urtiga	B-821	1
Wolf	Folha de urtiga	B821	1
Wolf	Folha de urtiga	P234605	10
Caelo	Folha de uva-ursi	12186506	3
Bombastus	Folha de uva-ursi	272297	8
Bombastus	Folha de uva-ursi	275491	3
Bombastus	Folha de uva-ursi	267926	1
Caelo	Folha de uva-ursi	11213011	3
Caelo	Folha de uva-ursi	20111210	1
Caelo	Folha de uva-ursi	11213010	1
Caelo	Folha de uva-ursi	13067802	3
Caelo	Folha de uva-ursi	12186503	1
Caelo	Folha de uva-ursi	15051303	1
Caelo	Folha de uva-ursi	4091301	1
Caelo	Folha de uva-ursi	13067805	6
Caelo	Folha de uva-ursi	5111301	1
Caelo	Folha de uva-ursi	12186504	1
Caelo	Folha de uva-ursi	17121306	1
Caelo	Folha de uva-ursi	4021407	1
Caelo	Folha de uva-ursi	15116201	1
Caelo	Folha de uva-ursi	17311305	1
Caelo	Folha de uva-ursi	17311308	1
Caelo	Folha de uva-ursi	1218602	1
Caelo	Folha de uva-ursi	280889	3
Caelo	Folha de uva-ursi	11213005	4
Caelo	Folha de uva-ursi	412A-01518	1
Caelo	Folha de uva-ursi	18304202	2
Caelo	Folha de uva-ursi	13067805-3390311080	1
Klenk	Folha de uva-ursi	2391b120314	2
Galke	Folha de uva-ursi	19936	3
Klenk	Folha de uva-ursi	2391B120314	6
Klenk	Folha de uva-ursi	2391B130328	9
Klenk	Folha de uva-ursi	2391B07030901	1
Caelo	Folha de uva-ursi	12186502	1
Sanacorp	Folha de uva-ursi	2391B110209	3
Klenk	Folha de uva-ursi	2391B120719	13
Caelo	Folha de verbena-limão, cortada	13037702	1
Caelo	Folha de verbena-limão, cortada	12137505	1
Caelo	Folha de verbena-limão, cortada	12137507	3
Caelo	Folha de verbena-limão, cortada	10018208	1
Klenk	Folha de verbena-limão, cortada	2411B110408	2
Wolf	Folha de verbena-limão, cortada	E-587	1
Wolf	Folha de verbena-limão, cortada	B-312	1
Wolf	Folha de verbena-limão, cortada	23635	1
AHD	Fosfato de sódio dibásico d…	112345013	1
Alliance	Fosfato de sódio dibásico d…	12256606	1
Caelo	Fosfato de sódio dibásico d…	1169315	1
Caelo	Fosfato de sódio dibásico d…	9302613	2
Caelo	Fosfato de sódio dibásico d…	11169315	1
Caelo	Fosfato de sódio dibásico d…	12345001	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fosfato de sódio dibásico d…	12345004	7
Caelo	Fosfato de sódio dibásico d…	12345007	3
Caelo	Fosfato de sódio dibásico d…	12345013	6
Caelo	Fosfato de sódio dibásico d…	71199028	1
Caelo	Fosfato de sódio dibásico d…	12345016	7
Caelo	Fosfato de sódio dibásico d…	83002059	1
Caelo	Fosfato de sódio dibásico d…	12256602	2
Caelo	Fosfato de sódio dibásico d…	11169309	3
Caelo	Fosfato de sódio dibásico d…	11169303	2
Caelo	Fosfato de sódio dibásico d…	12345025	1
Caelo	Fosfato de sódio dibásico d…	AKD7	1
Caesar&loretz,Anzag	Fosfato de sódio dibásico d…	12256606	3
Fagron	Fosfato de sódio dibásico d…	11K30-NO1	1
Fagron	Fosfato de sódio dibásico d…	2111E-01914	1
Fagron	Fosfato de sódio dibásico d…	1513I-01914	1
Fagron	Fosfato de sódio dibásico d…	B44888A	1
gebepharm	Fosfato de sódio dibásico d…	20160909-2	1
ICHTHYOL-GESELLSCHAFT	Fosfato de sódio dibásico d…	Caelo	1
Alliance healthcare	Fosfato de sódio monobásico…	12L05-N04	2
Bombastus	Fosfato de sódio monobásico…	11H04-N06	1
Fagron	Fosfato de sódio monobásico…	613I-01914	1
Fagron	Fosfato de sódio monobásico…	13D24-N12	2
Fagron	Fosfato de sódio monobásico…	13H01-B01	1
Caelo	Fosfato monobásico de sódio…	12109002	2
Caelo	Fosfato monobásico de sódio…	12109106	1
Caelo	Fosfato monobásico de sódio…	10135304	1
Caelo	Fosfato monobásico de sódio…	12109109	1
Caelo	Fosfato monobásico de sódio…	13028103	1
Caelo	Fosfato monobásico de sódio…	11109513	1
Caelo	Fosfato monobásico de sódio…	12109108	2
Caelo	Fosfato monobásico de sódio…	13028001	1
Caelo	Fosfato monobásico de sódio…	72006059	1
Gehe	Fosfato monobásico de sódio…	12109001	2
Jenne	Fosfato monobásico de sódio…	12109003	3
Phönix	Fosfato monobásico de sódio…	1302800,	1
Phönix	Fosfato monobásico de sódio…	13028101	1
Caelo	Fosfato monobásico de sódio…	13028003	1
Caelo	Fosfato tricálcico	1056303	1
EuRho	Fosfato tricálcico	13031203	1
Euro OTC	Fosfato tricálcico	1206002-01	3
Euro OTC	Fosfato tricálcico	1304025-01	2
Fagron	Fosfato tricálcico	12I13-N03	1
Caelo	Fruto da alcarávia, esmagada	12116904	3
Caelo	Fruto da alcarávia, esmagada	13367101	1
Galke	Fruto da alcarávia, esmagada	18943	1
Caelo	Fruto da sene tinnevelly	11003004	1
Caelo	Fruto da sene tinnevelly	11003009	2
Caelo	Fruto da sene tinnevelly	22061202	1
Caelo	Fruto da sene tinnevelly	110030009	1
Caelo	Fruto da sene tinnevelly	12267604	1
Caelo	Fruto da sene tinnevelly	12267609	3
Caelo	Fruto da sene tinnevelly	11003013	1
Caelo	Fruto da sene tinnevelly	122676707	1
Caelo	Fruto da sene tinnevelly	12267606	1
Caelo	Fruto da sene tinnevelly	12267602	2
Caelo	Fruto da sene tinnevelly	12267610	1
Caelo	Fruto da sene tinnevelly	12267608	1
Caelo	Fruto da sene tinnevelly	12267007	1
Caelo	Fruto da sene tinnevelly	12267201	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fruto da sene tinnevelly	17030712	1
Caelo	Fruto da sene tinnevelly	18240501	1
Caelo	Fruto da sene tinnevelly	18240505	1
Caelo	Fruto da sene tinnevelly	17030709	1
Caelo	Fruto da sene tinnevelly	17030708	1
Caelo	Fruto da sene tinnevelly	18240506	1
Caelo	Fruto da sene tinnevelly	12267605	1
Caesar & Loretz Gm…	Fruto da sene tinnevelly	11003012	1
Caesar & Loretz Gm…	Fruto da sene tinnevelly	11003014	1
Caesar & Loretz Gm…	Fruto da sene tinnevelly	12267601	2
Caesar & Loretz Gm…	Fruto da sene tinnevelly	12267603	1
Klenk	Fruto da sene tinnevelly	1041B120327	2
Caelo	Fruto de bérberis	11058320	1
Caelo	Fruto de bérberis	12217103	3
Caelo	Fruto de bérberis	12217106	1
Caelo	Fruto de bérberis	12217111	1
Caelo	Fruto de bérberis	12217113	2
Caelo	Fruto de bérberis	12217116	1
Caelo	Fruto de bérberis	16224202	1
Caelo	Fruto de bérberis	12217107	1
Caelo	Fruto de bérberis	1221707	1
Caelo	Fruto de bérberis	12217109	4
Berkel AHK	Fruto do agnocasto	14194401	4
Caelo	Fruto do agnocasto	11026309	1
Caelo	Fruto do agnocasto	12016909	4
Caelo	Fruto do agnocasto	12016902	1
Caelo	Fruto do agnocasto	12016908	1
Caelo	Fruto do agnocasto	12274010	10
Caelo	Fruto do agnocasto	12274008	1
Caelo	Fruto do agnocasto	12274009	3
Caelo	Fruto do agnocasto	12274014	1
Caelo	Fruto do agnocasto	13193401	2
Caelo	Fruto do agnocasto	13193403	1
Caelo	Fruto do agnocasto	1513546	1
Caelo	Fruto do agnocasto	13193407	1
Caelo	Fruto do agnocasto	13193410	2
Caelo	Fruto do agnocasto	14194408	1
Caelo	Fruto do agnocasto	15318702	1
Caelo	Fruto do agnocasto	15318705	1
Caelo	Fruto do agnocasto	15318718	1
Caelo	Fruto do agnocasto	9245308	1
Caelo	Fruto do agnocasto	12274002	1
Caelo	Fruto do agnocasto	13193406	1
Caelo	Fruto do agnocasto	15065105	1
Caelo	Fruto do agnocasto	11026318	1
Caelo	Fruto do agnocasto	12274013	2
Caelo	Fruto do agnocasto	3413A-03015	1
Caelo	Fruto do agnocasto	80175158	2
Caelo	Fruto do agnocasto	12016905	2
Caelo	Fruto do agnocasto	13193404	1
Gutenberg-Apotheke	Fruto do agnocasto	61765	1
Klenk	Fruto do agnocasto	A120803	1
Klenk	Fruto do agnocasto	7110N090701	1
Klenk	Fruto do agnocasto	A110614	3
Klenk	Fruto do agnocasto	7110A120803	1
Klenk	Fruto do agnocasto	7110A110614	2
Klenk	Fruto do agnocasto	A130613	1
Klenk	Fruto do agnocasto	7110N150121	1
Klenk	Fruto do agnocasto	7110A130613	1
Klenk	Fruto do agnocasto	12274007	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Fruto do agnocasto	12274006	3
Caelo	Fruto do agnocasto	12274003	4
Caelo	Fruto do agnocasto	12274012	1
Klenk	Fruto do aipo	7140A170210	1
Caelo	Fruto do cardamomo	11309110	1
Caelo	Fruto do cardamomo	13260502-3537411072	1
Klenk	Fruto do cardamomo	2750A110810	2
Klenk	Fruto do cardamomo	A110810	3
Klenk	Fruto do cardamomo	A130807	1
Caelo	Fruto do cardamomo	13026003	1
Bombastus	Fruto do cardo-mariano	296535	1
Bombastus	Fruto do cardo-mariano	296193	1
Bombastus	Fruto do cardo-mariano	299483	1
Bombastus	Fruto do cardo-mariano	269499	1
Bombastus	Fruto do cardo-mariano	280304	1
Bombastus	Fruto do cardo-mariano	278379	1
Bombastus	Fruto do cardo-mariano	282283	1
Bombastus	Fruto do cardo-mariano	282034	2
Bombastus	Fruto do cardo-mariano	279405	3
Bombastus	Fruto do cardo-mariano	277720	3
Bombastus	Fruto do cardo-mariano	278378	1
Bombastus	Fruto do cardo-mariano	284420	1
Bombastus	Fruto do cardo-mariano	13122013a	1
Caelo	Fruto do cardo-mariano	12189116	2
Caelo	Fruto do cardo-mariano	10270613	1
Caelo	Fruto do cardo-mariano	11126702	9
Caelo	Fruto do cardo-mariano	10270614	2
Caelo	Fruto do cardo-mariano	27111203	1
Caelo	Fruto do cardo-mariano	1126703	1
Caelo	Fruto do cardo-mariano	11126701	1
Caelo	Fruto do cardo-mariano	1126705	1
Caelo	Fruto do cardo-mariano	11126705	1
Caelo	Fruto do cardo-mariano	12189106	4
Caelo	Fruto do cardo-mariano	12189104	2
Caelo	Fruto do cardo-mariano	12189105	1
Caelo	Fruto do cardo-mariano	12189109	2
Caelo	Fruto do cardo-mariano	12189113	6
Caelo	Fruto do cardo-mariano	12189111	3
Caelo	Fruto do cardo-mariano	12189115	2
Caelo	Fruto do cardo-mariano	18111301	1
Caelo	Fruto do cardo-mariano	13326202	3
Caelo	Fruto do cardo-mariano	15409204	2
Caelo	Fruto do cardo-mariano	12198107	1
Caelo	Fruto do cardo-mariano	12189107	2
Caelo	Fruto do cardo-mariano	12189108	4
Caelo	Fruto do cardo-mariano	11126703	2
Caelo	Fruto do cardo-mariano	1289112	1
ebert u.jacobi	Fruto do cardo-mariano	287527	1
Galke	Fruto do cardo-mariano	22187	4
Klenk	Fruto do cardo-mariano	7180A090929	1
Klenk	Fruto do cardo-mariano	7180A120725	1
Klenk	Fruto do cardo-mariano	A120725	1
Klenk	Fruto do cardo-mariano	7180A130219	1
Klenk	Fruto do cardo-mariano	7180A132019	1
Klenk	Fruto do cardo-mariano	7180A110209	2
Caelo	Fruto do cardo-mariano	12189112	5
Akazie	Fruto do endro (Anethum gra...	20.09.2015	1
Caelo	Fruto do endro (Anethum gra...	12289901	1
Caelo	Fruto do endro (Anethum gra...	12038302	2
Caelo	Fruto do endro (Anethum gra...	12342901	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fruto do endro (Anethum gra…	12342904	7
Caelo	Fruto do endro (Anethum gra…	12342903	1
Caelo	Fruto do endro (Anethum gra…	12342908	2
Caelo	Fruto do endro (Anethum gra…	12038304	4
Caelo	Fruto do endro (Anethum gra…	9189003	1
Caelo	Fruto do endro (Anethum gra…	16040406	1
Caelo	Fruto do endro (Anethum gra…	12342906	2
Galke	Fruto do endro (Anethum gra…	22422	4
Hepart AG	Fruto do endro (Anethum gra…	L30057kbA	1
Klenk	Fruto do endro (Anethum gra…	2680A-120312	1
Klenk	Fruto do endro (Anethum gra…	2680A120312	8
Klenk	Fruto do endro (Anethum gra…	A120312	1
Klenk	Fruto do endro (Anethum gra…	2680A121211	3
Klenk	Fruto do endro (Anethum gra…	2680a120312	1
Kräuter Schulte	Fruto do endro (Anethum gra…	6363	1
Caelo	Fruto do endro (Anethum gra…	16348702	2
Caelo	Fruto do endro (Anethum gra…	16348707	1
Caelo	Fruto do endro (Anethum gra…	12342909	5
Wolf	Fruto do endro (Anethum gra…	E-501	1
Wolf	Fruto do endro (Anethum gra…	L30057	5
Wolf	Fruto do endro (Anethum gra…	23622	6
Caelo	Fruto do espinheiro-branco	11278202	1
Caelo	Fruto do espinheiro-branco	12326308	1
Caelo	Fruto do espinheiro-branco	13101402	2
Caelo	Fruto do espinheiro-branco	12326306	1
Caelo	Fruto do espinheiro-branco	13367203	1
Caelo	Fruto do espinheiro-branco	12326307	2
Klenk	Fruto do espinheiro-branco	2806B110818	2
Klenk	Fruto do espinheiro-branco	2806B121203	2
Caelo	Fruto do espinheiro-branco	12326304	1
Caelo	Fruto do sabugueiro	12267801	1
Gehe	Fruto do sabugueiro	12267807	1
Klenk	Fruto do sabugueiro	3010N120921	3
Fagron	Fucsina	12A03-N06	1
Fagron	Fucsina	12F28-N02	1
Fagron	Fucsina	12G18-N01	1
Fagron	Fucsina	13H23-M04	2
Fagron	Fucsina	13A30-N05	1
Lab.Offichem	Fumarato de dimetila	1605052.0393	1
Lab.Offichem	Fumarato de dimetila	1805043.0393	1
Lab.Offichem	Fumarato de dimetila	1808016.0393	1
Lab.Offichem	Fumarato de dimetila	1809012.0393	1
Lab.Offichem	Fumarato de dimetila	1910037.1814	1
Euro OTC	Fumarato monobásico de etil…	1510005-01	12
Lab.Offichem	Fumarato monobásico de etil…	1412007.0525	1
Lab.Offichem	Fumarato monobásico de etil…	1801004.0525	1
Lab.Offichem	Fumarato monobásico de etil…	1806023.0525	1
Fagron	Fumarato monobásico de etil…	14H27-B04-299502	6
Lab.Offichem	Fumarato monobásico de etil…	1604034.0527	1
Lab.Offichem	Fumarato monobásico de etil…	1805051.0527	1
Caelo	Fumitória	11101406	1
Caelo	Fumitória	11101410	1
Caelo	Fumitória	11101411	3
Caelo	Fumitória	11101413	3
Caelo	Fumitória	31081201	1
Caelo	Fumitória	7111201	1
Caelo	Fumitória	13202902	11
Caelo	Fumitória	13202905	2
Caelo	Fumitória	12103408	5
Caelo	Fumitória	12103405	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fumitória	11101408	1
Caelo	Fumitória	12103404	2
Caelo	Fumitória	12103407	6
Caelo	Fumitória	1320902	1
Caelo	Fumitória	72878477	1
Caelo	Fumitória	8312901	1
Gehe	Fumitória	12103402	2
Kenk / Phoenix	Fumitória	3881B111013	2
Klenk	Fumitória	B120410	1
Klenk	Fumitória	3881B100127	1

G

Supplier	Substance	Batch	Spectra
Anzag	Galium odoratum	12103504	2
Caelo	Galium odoratum	10375802	1
Caelo	Galium odoratum	4409M-01621	1
Caelo	Galium odoratum	52236077	1
Caelo	Galium odoratum	10375812	1
Caelo	Galium odoratum	18031304	1
Caelo	Galium odoratum	12103508	1
Caelo	Galium odoratum	12103510	1
Caelo	Galium odoratum	12103513	2
Caelo	Galium odoratum	12103509	1
Caelo	Galium odoratum	12103514	1
Gahlke	Galium odoratum	22100	1
Klenk	Galium odoratum	3601B090114	1
Klenk	Galium odoratum	B090114	3
Klenk	Galium odoratum	3601B140321	1
Kräuter-Schulte	Galium odoratum	52878	1
Caelo	Galium verum	10375707	2
Caelo	Galium verum	24101201	1
Caelo	Galium verum	11265102	9
Caelo	Galium verum	7011301	1
Caelo	Galium verum	2401311647	1
Caelo	Galium verum	22041303	1
Caelo	Galium verum	11265104	1
Caelo	Galium verum	14019202	1
Caelo	Galium verum	15029906	1
Caelo	Galium verum	11265103	5
Caelo	Galium verum	10375702	1
Caelo	Galium verum	12369002	3
Caelo	Galium verum	12369006	5
Caelo	Galium verum	12369007	3
Caesar&loretz,Phoenix	Galium verum	14019206	1
Caesar&loretz,Phoenix	Galium verum	14019215	1
Fagron	Galium verum	12369004	2
Galke	Galium verum	21942	2
Caelo	Galium verum	12369001	3
Klenk	Galium verum	3921B12030	1
Klenk	Galium verum	3921C130226	1
Caelo	Galium verum	11265106	3
Sanacorp	Galium verum	11265109	1
Sanacorp	Galium verum	12369003	8
Caelo	Gengibre	11325715	2
Caelo	Gengibre	11325716	1
Caelo	Gengibre	19121201	1
Caelo	Gengibre	11325719	3
Caelo	Gengibre	13100602	2
Caelo	Gengibre	13310604	4
Caelo	Gengibre	12180604	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Gengibre	13100604	1
Caelo	Gengibre	11325703	2
Caelo	Gengibre	11325712	1
Caelo	Gengibre	13100605	4
Caelo	Gengibre	13310602	2
Caelo	Gengibre	12164911-3368319002	1
Galke	Gengibre	20633	1
Galke	Gengibre	21766	2
Klenk	Gengibre	6951B110119	1
Klenk	Gengibre	6951B110822	1
Klenk	Gengibre	6951B100302	1
Klenk	Gengibre	6951B130110	1
Phönix	Gengibre	13310601	1
Richter	Gengibre	KR27992	1
Caelo	Gengibre, descascado, pulve…	12164901	1
Caelo	Gengibre, descascado, pulve…	13092013B	1
Caelo	Gengibre, descascado, pulve…	12164911	1
Klenk	Gengibre, descascado, pulve…	6954B16029	1
Klenk	Gengibre, descascado, pulve…	6954B170127	1
Klenk	Gengibre, descascado, pulve…	6954B110801	1
Klenk	Gengibre, descascado, pulve…	B121030	2
Klenk	Gengibre, descascado, pulve…	6954B130418	2
Klenk	Gengibre, descascado, pulve…	6954B121030	2
Klenk	Gengibre, descascado, pulve…	6954B160429	5
Klenk	Gengibre, descascado, pulve…	KS200260	1
Klenk	Gengibre, descascado, pulve…	6954B160929	2
C	Geranium robertianum, planta	11147810	3
Caelo	Geranium robertianum, planta	11147807	3
Caelo	Geranium robertianum, planta	11147804	1
Caelo	Geranium robertianum, planta	8121203	1
Caelo	Geranium robertianum, planta	11147813	2
Caelo	Geranium robertianum, planta	12319305	1
Caelo	Geranium robertianum, planta	12319304	2
Caelo	Geranium robertianum, planta	11147812	3
Caelo	Geranium robertianum, planta	12319302	1
Klenk	Geranium robertianum, planta	A110621	6
Klenk	Geranium robertianum, planta	3951A110621	7
Klenk	Geranium robertianum, planta	3951B121218	2
Klenk	Geranium robertianum, planta	3951B12118	1
Caelo	Ginseng siberiano, cortado	10381818	2
Caelo	Ginseng siberiano, cortado	12326703	1
Caelo	Ginseng siberiano, cortado	10381817	1
Caelo	Ginseng siberiano, cortado	12326707	1
Klenk	Ginseng siberiano, cortado	7011A121204	1
Klenk	Ginseng siberiano, cortado	7011A101206	1
Klenk	Ginseng siberiano, cortado	7011A110714	1
Caelo	Ginseng siberiano, cortado	12326701	1
Klenk	Girassol, cortado	1711I-07036	1
Klenk	Girassol, cortado	1701B091013	1
Caelo	Groselha	12272804	3
Caelo	Groselha	14212507	1
Galke	Groselha	21348	1
Klenk	Groselha	A121106	1
Klenk	Groselha	2990A110620	1
Caelo	Guaiaco (madeira)	11352001	1
Caelo	Guaiaco (madeira)	4011M-01778	1
Caelo	Guaiaco (madeira)	11352008	1
Caelo	Guaiaco (madeira)	8041401	1
Caelo	Guaiaco (madeira)	16136708	1
Caelo	Guaiaco (madeira)	10353102	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Guaiaco (madeira)	11352010	1
Caelo	Guaiaco (madeira)	14008203	1
Caelo	Guaiaco (madeira)	16136710	1
Caelo	Guaiaco (madeira)	16136706	1
Caelo	Guaiaco (madeira)	16136705	1
Caelo	Guaiaco (madeira)	11352012	1
sana 09.12.14 3,75	Guaiaco (madeira)	13343802	1

H

Supplier	Substance	Batch	Spectra
Caelo	Hena pulverizada	12122301	2
Caelo	Hena pulverizada	12122310	3
Caelo	Hena pulverizada	13262803	2
Caelo	Hena pulverizada	12267311	1
Klenk	Hena pulverizada	20747A111004	1
Klenk	Hena pulverizada	2074A111004	1
Caelo	Hera-terrestre	11052315	1
Caelo	Hera-terrestre	11052314	1
Caelo	Hera-terrestre	11374611	2
Caelo	Hera-terrestre	11374615	1
Caelo	Hera-terrestre	11374606	1
Caelo	Hera-terrestre	11374602	1
Caelo	Hera-terrestre	11374609	1
Caelo	Hera-terrestre	11052318	2
Gutenberg-Apotheke	Hera-terrestre	11374610	3
Klenk	Hera-terrestre	3991B110304	1
Klenk	Hera-terrestre	3991B130502	2
Phönix	Hera-terrestre	11374608	1
Richter	Hera-terrestre	s99/09	1
Caelo	Herniária	11104507	8
Caelo	Herniária	13007502	2
Caelo	Herniária	13007505	1
Caelo	Herniária	14005303	1
Caelo	Herniária	14005305	3
Caelo	Herniária	14197204	1
Caelo	Herniária	1711924	1
Caelo	Herniária	16292809	1
Caelo	Herniária	16292801	1
Caelo	Herniária	11104505	1
Caelo	Herniária	13007507	7
Klenk	Herniária	4011B131115	3
Klenk	Herniária	4011B121207	2
Audor Pharma	Hialuronato de sódio	AP30101305H	2
Audor Pharma	Hialuronato de sódio	AP30101404H	1
Audor Pharma	Hialuronato de sódio	A0397074	1
Audor Pharma	Hialuronato de sódio	AP30101505H	1
Audor Pharma	Hialuronato de sódio	AP30101404H	1
Caelo	Hialuronato de sódio	17234702	1
Caelo	Hialuronato de sódio	1263303	1
Caelo	Hialuronato de sódio	14188702	1
Caelo	Hialuronato de sódio	14364706	2
Caelo	Hialuronato de sódio	16246703	1
Caelo	Hialuronato de sódio	15204901	1
Caelo	Hialuronato de sódio	15204903	3
Caelo	Hialuronato de sódio	193031002	1
Caelo	Hialuronato de sódio	17234701	1
Caelo	Hialuronato de sódio	21002684002	4
Caelo	Hialuronato de sódio	15448803	1
Calo/AHD	Hialuronato de sódio	14364704	1
Euro OTC	Hialuronato de sódio	L1710023-02	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Hialuronato de sódio	L1907021-01	1
Euro OTC	Hialuronato de sódio	L1512025-01	2
Euro OTC	Hialuronato de sódio	L2103023-01	1
Fagron	Hialuronato de sódio	L1311012-01	1
Fisher Scientific	Hialuronato de sódio	A0387534	1
Caelo	Hialuronato de sódio	2100131002	1
Caelo	Hialuronato de sódio	21000131002	1
Fagron	Hidróxido de cálcio	12J18-N01	1
Fagron	Hidróxido de cálcio	13D26-N14	1
Gehe	Hidróxido de cálcio	12F08-N02	3
Caelo	Hidróxido de potássio	12057905	1
Caelo	Hidróxido de potássio	11165708	1
Caelo	Hidróxido de potássio	17091202	1
Caelo	Hidróxido de potássio	12057912	2
Caelo	Hidróxido de potássio	12057908	2
Caelo	Hidróxido de potássio	12057906	1
Caelo	Hidróxido de potássio	12382606	2
Caelo	Hidróxido de potássio	11165705	1
Caelo	Hidróxido de potássio	12382611	1
Caelo	Hidróxido de potássio	27111310	1
Caelo	Hidróxido de potássio	13275201	2
Caelo	Hidróxido de potássio	12382601	2
Caelo	Hidróxido de potássio	13275207	1
Caesar & Loretz Gm…	Hidróxido de potássio	12057902	2
Caelo	Hidróxido de potássio	12382603	4
Caelo	Hidróxido de sódio	15312102	1
Caelo	Hidróxido de sódio	11070821	1
Fagron	Hidróxido de sódio	12E02-N15	1
Fagron	Hidróxido de sódio	13F06-N02	3
Fagron	Hidróxido de sódio	13k22-no5	1
Caelo	Hidróxido de sódio	12368105	1

K

Supplier	Substance	Batch	Spectra
Caelo	Kelp, cortado	11351109	1
Caelo	Kelp, cortado	14071502	1
Caelo	Kelp, cortado	11352209	1
Klenk	Kelp, cortado	1051A110920	1
Caelo	Kelp, cortado	280172	4
Sanacorp	Kelp, cortado	11351105	1

L

Supplier	Substance	Batch	Spectra
Caelo	Lamium album	11371702	1
Caelo	Lamium album	11371706	3
Caelo	Lamium album	11371709	2
Caelo	Lamium album	11371711	2
Caelo	Lamium album	11371705	1
Caelo	Lamium album	11371712	1
Caelo	Lamium album	11371703	1
Galke	Lamium album	22253	2
Galke	Lamium album	19706	1
-	Laranja-amarga (Citrus aura…	2011A-01445	1
Caelo	Laranja-amarga (Citrus aura…	11049212	1
Caelo	Laranja-amarga (Citrus aura…	12266703	2
Caelo	Laranja-amarga (Citrus aura…	11049202	1
Caelo	Laranja-amarga (Citrus aura…	12266608	6
Caelo	Laranja-amarga (Citrus aura…	2712E-01445	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Laranja-amarga (Citrus aura…	12266609	1
Caelo	Laranja-amarga (Citrus aura…	6051301	1
Caelo	Laranja-amarga (Citrus aura…	12266708	1
Caelo	Laranja-amarga (Citrus aura…	13067903	2
Caelo	Laranja-amarga (Citrus aura…	12266705	1
Caelo	Laranja-amarga (Citrus aura…	12266614	1
Caelo	Laranja-amarga (Citrus aura…	13352701	1
Caelo	Laranja-amarga (Citrus aura…	12266707	1
Caelo	Laranja-amarga (Citrus aura…	12266605	1
Caelo	Laranja-amarga (Citrus aura…	12266611	1
Caelo	Laranja-amarga (Citrus aura…	12266608	2
Caelo	Laranja-amarga (Citrus aura…	12266605	1
Caelo	Laranja-amarga (Citrus aura…	12266611	1
Caelo	Laranja-amarga (Citrus aura…	13352701-3518411022	1
Hepart AG	Laranja-amarga (Citrus aura…	B120822	1
Klenk	Laranja-amarga (Citrus aura…	1201B120822	1
Klenk	Laranja-amarga (Citrus aura…	1201B110809	1
Klenk	Laranja-amarga (Citrus aura…	3613m-01445	1
Bombastus	Laranja-amarga, casca	278233	4
Bombastus	Laranja-amarga, casca	274240	3
Caelo	Laranja-amarga, casca	12239203	3
Caelo	Laranja-amarga, casca	12067402	1
Caelo	Laranja-amarga, casca	17111201	1
Caelo	Laranja-amarga, casca	12067405	1
Caelo	Laranja-amarga, casca	4312M-01531	1
Caelo	Laranja-amarga, casca	13049001	1
Caelo	Laranja-amarga, casca	21101302	1
Caelo	Laranja-amarga, casca	27011403	1
Klenk	Laranja-amarga, casca	511B110321	2
Klenk	Laranja-amarga, casca	2711B111207	1
Klenk	Laranja-amarga, casca	511B120830	4
Klenk	Laranja-amarga, casca	511A110411	1
Klenk	Laranja-amarga, casca	B120830	1
Klenk	Laranja-amarga, casca	C130226	3
Klenk	Laranja-amarga, casca	511C130226	1
Klenk	Laranja-amarga, casca	3613M-01531	1
kräuter schulte	Laranja-amarga, casca	51265	1
Caelo	Leonurus cardiaca	5061203	1
Caelo	Leonurus cardiaca	12376403	1
Caelo	Leonurus cardiaca	12376408	2
Caelo	Leonurus cardiaca	12376407	1
Caelo	Leonurus cardiaca	11293004	1
Gehe	Leonurus cardiaca	12231502	3
Klenk	Leonurus cardiaca	4071A-100707	1
Phönix	Leonurus cardiaca	12231503	2
Euro OTC	Levedura de cromo 0,2%	L1311026-01	1
Bombastus	Levisticum officinale	273001	1
Caelo	Levisticum officinale	11181609	3
Caelo	Levisticum officinale	12189001	1
Caelo	Levisticum officinale	11181611	3
Caelo	Levisticum officinale	4312M-02150	1
Caelo	Levisticum officinale	12169007	1
Caelo	Levisticum officinale	12169009	1
Caelo	Levisticum officinale	12169012	1
Caelo	Levisticum officinale	13385005	1
Caelo	Levisticum officinale	12189002	1
Caelo	Levisticum officinale	107063	1
Caelo	Levisticum officinale	12169008	4
Caelo	Levisticum officinale	12169006	3
Caelo	Levisticum officinale	12169002	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Levisticum officinale	12169010	2
Klenk	Levisticum officinale	6371A080508	1
Klenk	Levisticum officinale	B110228	1
Klenk	Levisticum officinale	B121029	1
Klenk	Levisticum officinale	6371B-121029	1
Klenk	Levisticum officinale	6371B121029	3
Caelo	Licopódio (Lycopodium clavatum)	11255012	2
Bahnhof-Apotheke	Licopódio (Lycopodium clavatum)	17-121112	1
Caelo	Licopódio (Lycopodium clavatum)	11255003	1
Caelo	Licopódio (Lycopodium clavatum)	9378812	1
Caelo	Licopódio (Lycopodium clavatum)	11255005	3
Caelo	Licopódio (Lycopodium clavatum)	11255008	12
Caelo	Licopódio (Lycopodium clavatum)	11255009	3
Caelo	Licopódio (Lycopodium clavatum)	11255011	5
Caelo	Licopódio (Lycopodium clavatum)	11255014	7
Caelo	Licopódio (Lycopodium clavatum)	11255010	1
Caelo	Licopódio (Lycopodium clavatum)	11255016	2
Caelo	Licopódio (Lycopodium clavatum)	11255018	1
Caelo	Licopódio (Lycopodium clavatum)	13101501	1
Caelo	Licopódio (Lycopodium clavatum)	1310502	1
Caesar/Noweda	Licopódio (Lycopodium clavatum)	1255008	1
Finze	Licopódio (Lycopodium clavatum)	9378803	1
Galke	Licopódio (Lycopodium clavatum)	16913	3
Klenk	Licopódio (Lycopodium clavatum)	4111B120220	1
Klenk	Licopódio (Lycopodium clavatum)	4111B110428	1
Caelo	Licopódio (Lycopodium clavatum)	11255017	6
Sanacorp	Licopódio (Lycopodium clavatum)	13101502	2
Akazie	Linhaça	20.09.2015	2
Anzag	Linhaça	12137105	1
Bombastus	Linhaça	1610	1
Bombastus	Linhaça	269500	1
Bombastus	Linhaça	278457	6
Bombastus	Linhaça	274032	1
Bombastus	Linhaça	282734	3
Bombastus	Linhaça	295376	1
Caelo	Linhaça	15061201	1
Caelo	Linhaça	12092102	4
Caelo	Linhaça	11365508	1
Caelo	Linhaça	11365507	1
Caelo	Linhaça	12092103	3
Caelo	Linhaça	12321601	1
Caelo	Linhaça	12092104	2
Caelo	Linhaça	28051303	1
Caelo	Linhaça	12321602	4
Caelo	Linhaça	12321604	2
Caelo	Linhaça	11199006	1
Caelo	Linhaça	1232006	1
Caelo	Linhaça	12382006	3
Caelo	Linhaça	12321607	1
Caelo	Linhaça	18111302	1
Caelo	Linhaça	12321606	2
Caelo	Linhaça	13262702	1
Caelo	Linhaça	13296702	3
Caelo	Linhaça	13262703	3
Caelo	Linhaça	28051403	1
Caelo	Linhaça	1326703	2
Caelo	Linhaça	7370A131104	1
Caelo	Linhaça	13140305	1
Caelo	Linhaça	13412804	1
Caelo	Linhaça	13262704	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Linhaça	15053702	1
Caelo	Linhaça	13296707	1
Caelo	Linhaça	15006005	1
Caelo	Linhaça	15006605	1
Caelo	Linhaça	15321902	1
Caelo	Linhaça	21081703	1
Caelo	Linhaça	3923	1
Caelo	Linhaça	17067203	1
Caelo	Linhaça	12382002	2
Caelo	Linhaça	16355404	1
Caelo	Linhaça	18007801	2
Caelo	Linhaça	18145601	1
Caelo	Linhaça	13296705	5
Caelo	Linhaça	16040002	1
Caelo	Linhaça	17067204	1
Caelo	Linhaça	16040005	1
Caelo	Linhaça	12186901	2
Caelo	Linhaça	16040001	1
Caelo	Linhaça	16011403	3
Caelo	Linhaça	15006601	2
Caelo	Linhaça	15006607	1
Caelo	Linhaça	16355401	2
Caelo	Linhaça	4713U02240	1
Caelo	Linhaça	15006602	2
Caelo	Linhaça	7307A170619	2
Caelo	Linhaça	3615A-02240	1
Caelo	Linhaça	18145603	2
Caelo	Linhaça	11199003	1
Caelo	Linhaça	7307A141201	3
Fiebig	Linhaça	16011405	4
Finze	Linhaça	3607E-02240	1
Gehe	Linhaça	18145605	1
Hedinger	Linhaça	16011402	1
Heinrich Kle/Sanacor	Linhaça	7307A170111	3
Klenk	Linhaça	1910212240	1
Klenk	Linhaça	903312240	1
Klenk	Linhaça	7300A111107	4
Klenk	Linhaça	7308A111107	3
Klenk	Linhaça	7300A130110	7
Klenk	Linhaça	1913Q-02240	1
Klenk	Linhaça	A130110	1
Klenk	Linhaça	7307A130722	5
Klenk	Linhaça	7307A-130722	1
Klenk	Linhaça	7300A140526	1
Klenk	Linhaça	7307A160414	4
Klenk	Linhaça	7308A150710	2
Klenk	Linhaça	7300A170306	7
Klenk	Linhaça	7300A180523	2
Klenk	Linhaça	7300A170306-1	1
Klenk	Linhaça	7300A141201	6
Klenk	Linhaça	7308A150414	2
Klenk	Linhaça	7307A150710	6
Klenk	Linhaça	7307A170110	2
Klenk	Linhaça	7307A130124	1
Klenk	Linhaça	7307a131104	1
Klenk	Linhaça	7307A140526	3
Klenk	Linhaça	7308A130110	4
Klenk	Linhaça	2002285	1
Klenk	Linhaça	7307A131104	8
Klenk	Linhaça	7307A-130110	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Linhaça	3707A140526	1
Klenk	Linhaça	7500A140556	1
Klenk	Linhaça	7300A130722	8
Midas	Linhaça	7308A161208	1
Noweda	Linhaça	7307A111107	7
Klenk	Linhaça	7307a111107	1
Klenk	Linhaça	7307A121212	1
Caelo	Linhaça	12382004	1
Klenk	Linhaça	7307A131021	1
Phonix	Linhaça	13296703	3
Klenk	Linhaça	7307A150414	1
Caelo	Linhaça	16355402	7
Klenk	Linhaça	7307A130110	15

M

Supplier	Substance	Batch	Spectra
Caelo	Maçã selvagem, doce	11229805	1
Caelo	Maçã, cortada	12227301	1
Klenk	Maçã, cortada	A120302	3
Fagron	Macrogol 6000, pó	14J17-B01	1
Fagron	Macrogol 6000, pó	12J22-N02	1
Fagron	Macrogol 6000, pó	11G14-N03	1
Anzag ek:8.77EUR 30.08.12	Maná	11308904	2
Caelo	Maná	11308901	2
Caelo	Maná	11308909	2
Caelo	Maná	25111301	1
Caelo	Maná	11041401	1
Caelo	Maná	11061404	1
Caelo	Maná	25071403	1
Caelo	Maná	28101404	1
Caelo	Maná	13041712	1
Caelo	Maná	15219010	3
Caelo	Maná	15111738	1
Caelo	Maná	11308907	2
Caelo	Maná	13127003	5
Caelo	Maná	11308911	2
Caelo	Maná	15219005	1
Caelo	Maná	14001303	3
Caelo	Maná	14001310	3
Caelo	Maná	15219003	3
Caelo	Maná	15219008	3
Klenk	Maná	5221A110817	1
Klenk	Maná	5221A140210	4
Klenk	Maná	5221A150107	2
Caelo	Maná	15219012	1
Klenk	Maná	5221A120509	10
Caelo	Maná	15219009	1
Caelo	Maná, pulverizado	11308802	2
Caelo	Maná, pulverizado	11003611	1
Caelo	Maná, pulverizado	11071311	1
Caelo	Maná, pulverizado	15101306	1
Caelo	Maná, pulverizado	15101312	1
Caelo	Maná, pulverizado	11308807	1
Caelo	Maná, pulverizado	14001402	1
Caelo	Maná, pulverizado	14001408	1
Galke	Maná, pulverizado	20669	1
Galke	Maná, pulverizado	19784	1
Noweda	Maná, pulverizado	11170102	1
Klenk	Manjericão, triturado	3632A110201	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Manjericão, triturado	12066404	1
Caelo	Manjericão, triturado	12007010	4
Caelo	Manjericão, triturado	12007008	2
Caelo	Manjericão, triturado	13048601	2
Caelo	Manjericão, triturado	13048605	1
Caelo	Manjericão, triturado	13048605-3519411022	1
Klenk	Manjericão, triturado	3632A120502	4
Klenk	Manjericão, triturado	A110201	1
Klenk	Manjericão, triturado	A120502	1
Klenk	Manjericão, triturado	3632a120502	1
VDL	Manjericão, triturado	12007004	1
Caelo	Manjerona	12168901	3
Caelo	Manjerona	11212711	3
Caelo	Manjerona	12168903	10
Caelo	Manjerona	12168905	2
Caelo	Manjerona	12168904	1
Caelo	Manjerona	12168908	6
Caelo	Manjerona	6051302	1
Caelo	Manjerona	12168907	3
Caelo	Manjerona	12168912	1
Caelo	Manjerona	27011402	1
Caelo	Manjerona	11212707	1
Caelo	Manjerona	12168906	1
Caelo	Manjerona	13113304	3
Caelo	Manjerona	12168909	6
Caelo	Manjerona	13113303	3
Caelo	Manjerona	12168902	1
Caelo	Manjerona	12168910	8
Caelo	Manjerona	9292602	1
Caesar&loretz,Phoenix	Manjerona	14181005	1
Galke	Manjerona	22401	1
Galke	Manjerona	23241	1
Klenk	Manjerona	4881A101025	15
Klenk	Manjerona	A101025	2
Klenk	Manjerona	4881A1311105	1
Klenk	Manjerona	4881a101025	1
Klenk	Manjerona	12345678	1
Noweda	Manjerona	4881A100929	3
Wolf	Manjerona	163516	1
Wolf	Manjerona	B163516	6
Wolf	Manjerona	P232243	9
an	Maracujá, planta	13141212	1
Anzag	Maracujá, planta	1207211669	1
Caelo	Maracujá, planta	11049116	4
Caelo	Maracujá, planta	12031703	2
Caelo	Maracujá, planta	12031704	1
Caelo	Maracujá, planta	11049108	1
Caelo	Maracujá, planta	1011A-01669	1
Caelo	Maracujá, planta	12031701	1
Caelo	Maracujá, planta	12031715	7
Caelo	Maracujá, planta	12031716	3
Caelo	Maracujá, planta	12031712	1
Caelo	Maracujá, planta	12101301	1
Caelo	Maracujá, planta	13141201	1
Caelo	Maracujá, planta	15085105	1
Caelo	Maracujá, planta	12031706	3
Caelo	Maracujá, planta	11049111	1
Caelo	Maracujá, planta	13141202	7
Caelo	Maracujá, planta	12031710	13
Caelo	Maracujá, planta	12031705	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Maracujá, planta	13141205	4
Caelo	Maracujá, planta	12031714	2
Caelo	Maracujá, planta	12031717	9
Caelo	Maracujá, planta	13141203	2
Klenk	Maracujá, planta	4231A120329	2
Klenk	Maracujá, planta	A120329	2
Klenk	Maracujá, planta	4231A-110913	1
Caelo	Margarida, flor	11103201	2
Caelo	Margarida, flor	11068308	1
Caelo	Margarida, flor	1210a120215	2
Caelo	Margarida, flor	12133703	1
Caelo	Margarida, flor	12133704	1
Caelo	Margarida, flor	12133705	1
Caelo	Margarida, flor	11103203	2
Hepart AG	Margarida, flor	A130307	1
Kenk / Phoenix	Margarida, flor	1210A130307	4
Klenk	Margarida, flor	A130705	1
Klenk	Margarida, flor	1210A110223	1
Klenk	Margarida, flor	1210A120215	4
Klenk	Margarida, flor	1210a071301	1
-	Meliloto	811Q-01664	1
Anzag ek:3,13EUR 15.09.12	Meliloto	11307605	4
Caelo	Meliloto	8061204	1
Caelo	Meliloto	19071201	1
Caelo	Meliloto	24081202	1
Caelo	Meliloto	11307606	6
Caelo	Meliloto	11307601	1
Caelo	Meliloto	12231703	3
Caelo	Meliloto	12289202	8
Caelo	Meliloto	11307607	1
Caelo	Meliloto	122891202	1
Caelo	Meliloto	12289203	5
Caelo	Meliloto	25091301	1
Caelo	Meliloto	22111303	1
Caelo	Meliloto	12289206	1
Caelo	Meliloto	12289207	1
Caelo	Meliloto	12289201	1
Caelo	Meliloto	12231701	3
Caelo	Meliloto	107063	1
Caelo	Meliloto	12289205	4
Gehe	Meliloto	110324	1
Klenk	Meliloto	4151A110324	8
Klenk	Meliloto	4151A120912	1
Klenk	Meliloto	A110324	6
Phönix	Meliloto	1237903	1
Bahnhof-Apotheke	Melilotus vulgaris	13-121105	1
Caelo	Melilotus vulgaris	11099912	1
Caelo	Melilotus vulgaris	25101202	1
Caelo	Melilotus vulgaris	11099914	1
Caelo	Melilotus vulgaris	11099916	1
Caelo	Melilotus vulgaris	11099909	1
Caelo	Melilotus vulgaris	12317102	3
Caelo	Melilotus vulgaris	1231702	1
Caelo	Melilotus vulgaris	12317108	3
Caelo	Melilotus vulgaris	12317107	14
Caelo	Melilotus vulgaris	13097302	9
Caelo	Melilotus vulgaris	12317110	2
Caelo	Melilotus vulgaris	13099205	1
Caelo	Melilotus vulgaris	14121301	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melilotus vulgaris	13097301	1
Caelo	Melilotus vulgaris	11099902	1
Caelo	Melilotus vulgaris	12317104	10
Caelo	Melilotus vulgaris	3713E-01459	1
Caelo	Melilotus vulgaris	3713F-01459	1
Caelo	Melilotus vulgaris	12317101	8
Caelo	Melilotus vulgaris	12371707	1
Galke	Melilotus vulgaris	21926	1
Klenk	Melilotus vulgaris	A130304	1
Klenk	Melilotus vulgaris	10192103	1
Klenk	Melilotus vulgaris	1400A120116	1
Nachprüfung	Melilotus vulgaris	1911E01459	1
Caelo	Melilotus vulgaris	11099915	1
AHD	Mentha spicata, folha	14343404	1
Caelo	Mentha spicata, folha	12133901	3
Caelo	Mentha spicata, folha	1512Q-01505	1
Caelo	Mentha spicata, folha	11037409+110374	1
Caelo	Mentha spicata, folha	12133906	2
Caelo	Mentha spicata, folha	13105001	10
Caelo	Mentha spicata, folha	12376706	1
Caelo	Mentha spicata, folha	12133909	1
Caelo	Mentha spicata, folha	13105003	1
Fagron	Midazolam	14C12-B31-313222	1
Fagron	Midazolam	16J03-B09-326963	1
Klenk	Mil-folhas (Achillea millef…	4181A121130	1
Caelo	Mil-folhas (Achillea millef…	12267702	1
Caelo	Mil-folhas (Achillea millef…	12363005	5
Caelo	Mil-folhas (Achillea millef…	13350507	1
Caelo	Mil-folhas (Achillea millef…	12267703	2
Caelo	Mil-folhas (Achillea millef…	12363002	6
Caelo	Mil-folhas (Achillea millef…	12338306	1
Caelo	Mil-folhas (Achillea millef…	70139427	1
Klenk	Mil-folhas (Achillea millef…	A110816	3
Caelo	Mirra	11276810	1
Caelo	Mirra	11276806	1
Caelo	Mirra	11277111	1
Caelo	Mirra	12269901	2
Caelo	Mirra	12269907	1
Caelo	Mirra	25071404	1
Caelo	Mirra	28101401	1
Caelo	Mirra	30121413	1
Caelo	Mirra	12269913	1
Caelo	Mirra	14347509	1
Caelo	Mirra	15021410	1
Caelo	Mirra	15312606	1
Caelo	Mirra	12269904	4
Caelo	Mirra	14244602	1
Caelo	Mirra	11277111	1
Caelo	Mirra	12244404	1
Caelo	Mirra	12244406	1
Caelo	Mirra	11277105	1
Caelo	Mirra	13108701	2
Caelo	Mirra	15021402	1
Klenk	Mirra	3351A121004	1
Klenk	Mirra	3351A130902	1
Klenk	Mirra	3351A120514	1
Klenk	Mirra	3355B140723	1
Klenk	Mirra	3355B161010	1
Klenk	Mirra	3351A160330	4
phönix	Mirra	15021411	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
phönix	Mirra	3351a160330	1
Anzag	Mirtilo seco	2910N120921	2
Cae	Mirtilo seco	212172	1
Caelo	Mirtilo seco	13130504	1
Caelo	Mirtilo seco	12183701	2
Caelo	Mirtilo seco	26061301	1
Caelo	Mirtilo seco	10265601	1
Caelo	Mirtilo seco	18101307	1
Caelo	Mirtilo seco	13130501	1
Caelo	Mirtilo seco	10273708	1
Caelo	Mirtilo seco	10273709	1
Caelo	Mirtilo seco	10265603	1
Caelo	Mirtilo seco	10273711	1
Caelo	Mirtilo seco	12183704	4
Fiebig 05.11.12 ek...	Mirtilo seco	2910A120410	1
Klenk	Mirtilo seco	2910N110304	5
Klenk	Mirtilo seco	2010N110304	1
Klenk	Mirtilo seco	2910A090717	1
Klenk	Mirtilo seco	2910N130131	11
Klenk	Mirtilo seco	N130131	2
Klenk	Mirtilo seco	N121022	1
Klenk	Mirtilo seco	2910n130131	1
Klenk	Mirtilo seco	910N130131	1
Klenk	Mirtilo seco	2910n110304	1
Klenk	Mirtilo seco	2910N121022	7
Caelo	Monoestearato de glicerol d...	11160012	1
Noweda	Monoestearato de glicerol d...	11160010	1
-	Musgo-da Islândia	4711E-01774	1
Anzag ek: 15,60 20...	Musgo-da Islândia	11101605	1
Bombastus	Musgo-da Islândia	13357802	1
Caelo	Musgo-da Islândia	13350805	4
Caelo	Musgo-da Islândia	11101601	1
Caelo	Musgo-da Islândia	11101607	8
Caelo	Musgo-da Islândia	12197002	1
Caelo	Musgo-da Islândia	4912E-01774	1
Caelo	Musgo-da Islândia	12187002	1
Caelo	Musgo-da Islândia	11053916	1
Caelo	Musgo-da Islândia	12187103	1
Caelo	Musgo-da Islândia	12187106	3
Caelo	Musgo-da Islândia	12187109	4
Caelo	Musgo-da Islândia	12187107	1
Caelo	Musgo-da Islândia	13350803	4
Caelo	Musgo-da Islândia	12382806	1
Caelo	Musgo-da Islândia	13350807	4
Caelo	Musgo-da Islândia	14304402	1
Caelo	Musgo-da Islândia	14304401	1
Caelo	Musgo-da Islândia	14304407	2
Caelo	Musgo-da Islândia	15297601	1
Caelo	Musgo-da Islândia	711906	1
Caelo	Musgo-da Islândia	15297606	1
Caelo	Musgo-da Islândia	18078207	1
Caelo	Musgo-da Islândia	12187102	21
Caelo	Musgo-da Islândia	12187108	4
Caelo	Musgo-da Islândia	15297605	4
Caelo	Musgo-da Islândia	14304403	2
Caelo	Musgo-da Islândia	11053911	1
Caelo	Musgo-da Islândia	1287102	1
Caelo	Musgo-da Islândia	14304409	6
Caelo	Musgo-da Islândia	9052804	2
Caelo	Musgo-da Islândia	15297603	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
caesar&loretz,Phönix	Musgo-da Islândia	14304404	3
Galke	Musgo-da Islândia	12369	1
Gehe	Musgo-da Islândia	11101603	1
Gehe	Musgo-da Islândia	11053915	1
Gehe	Musgo-da Islândia	18079703	1
Klenk	Musgo-da Islândia	5191N110609	1
Klenk	Musgo-da Islândia	5191A140828	2
noweda	Musgo-da Islândia		1
Phönix	Musgo-da Islândia	12187104	3

N

Supplier	Substance	Batch	Spectra
Caelo	Nitrato de econazol	ECN140301	1
Fagron	Nitrato de econazol	11K07-N03	1
Fagron	Nitrato de econazol	13D22-N06	1
Fagron	Nitrato de econazol	11F09-N16	1
Fagron	Nitrato de econazol	12F18-N05	1
Fagron	Nitrato de econazol	14G22-B07-306926	1
Caelo	Noz moscada	12376805	1
Caelo	Noz moscada	12376802	2
Caelo	Noz-moscada, pulverizada (e...	12102305	2
Galke	Noz-moscada, pulverizada (e...	22739	1
Klenk	Noz-moscada, pulverizada (e...	A130304	2
Klenk	Noz-moscada, pulverizada (e...	7325A120903	2
Klenk	Noz-moscada, pulverizada (e...	7325A130304	1
Klenk	Noz-moscada, pulverizada (e...	7325A130515	1

O

Supplier	Substance	Batch	Spectra
Caelo	Olíbano	12120005	5
Caelo	Olíbano	10349210	1
Caelo	Olíbano	10349213	1
Caelo	Olíbano	12120008	2
Caelo	Olíbano	13112801	5
Caelo	Olíbano	13112809	2
Caelo	Olíbano	4614M-02030	1
Caelo	Olíbano	15140810	1
Caelo	Olíbano	802929	1
Caelo	Olíbano	15140809	2
Caelo	Olíbano	15140805	2
Caelo	Olíbano	15140804	1
Caelo	Olíbano	12120006	3
Caelo	Olíbano	13112803	1
Caelo	Olíbano	13112807	1
Caelo	Olíbano	14107803	2
Caelo	Olíbano	12120012-3421310191	1
Caelo	Olíbano	13112803-3494411030	1
Fagron	Olíbano		1
Gahlke	Olíbano	21949	1
vedono	Olíbano	12120009	5
vedono	Olíbano	12120012	1
Caelo	Orégano	12360904	1
Caelo	Orégano	11340705	1
Caelo	Orégano	11340708	1
Caelo	Orégano	11340709	1
Caelo	Orégano	12360901	6
Caelo	Orégano	11340703	2
Caelo	Orégano	12360902	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Orégano	4221A120315	2
Euro OTC	Orotato de cálcio di-hidratado	1401006-01	1
Euro OTC	Orotato de cálcio di-hidratado	1203037-01	2

P

Supplier	Substance	Batch	Spectra
Alfred Galke	Pé-de-leão	20921	1
Caelo	Pé-de-leão	13141105	3
Anzag ek: 6,39 11…	Pé-de-leão	11182806	6
Bombastus	Pé-de-leão	279070	5
Bahnhof-Apotheke	Pé-de-leão	17-121107	1
Bombastus	Pé-de-leão	272021	5
Bombastus	Pé-de-leão	276173	3
Bombastus	Pé-de-leão	278889	1
Bombastus	Pé-de-leão	282032	2
Bombastus	Pé-de-leão	14066007	1
Bombastus	Pé-de-leão	521203995	1
Bombastus	Pé-de-leão	266404	1
Bombastus	Pé-de-leão	231013B	1
Caelo	Pé-de-leão	1100912	1
Caelo	Pé-de-leão	11002906	5
Caelo	Pé-de-leão	11182801	3
Caelo	Pé-de-leão	11182804	3
Caelo	Pé-de-leão	1406211616	1
Caelo	Pé-de-leão	11182807	2
Caelo	Pé-de-leão	21081203	1
Caelo	Pé-de-leão	11182805	1
Caelo	Pé-de-leão	11063605	1
Caelo	Pé-de-leão	11182808	1
Caelo	Pé-de-leão	12153301	3
Caelo	Pé-de-leão	8121201	1
Caelo	Pé-de-leão	12153303	7
Caelo	Pé-de-leão	12153305	25
Caelo	Pé-de-leão	12153307	3
Caelo	Pé-de-leão	12342901	1
Caelo	Pé-de-leão	5041301	1
Caelo	Pé-de-leão	125306	1
Caelo	Pé-de-leão	H-040513-2	1
Caelo	Pé-de-leão	13141103	36
Caelo	Pé-de-leão	2081304	1
Caelo	Pé-de-leão	intch:318080	1
Caelo	Pé-de-leão	3613M01616	1
Caelo	Pé-de-leão	13091304	1
Caelo	Pé-de-leão	13141106	8
Caelo	Pé-de-leão	9011405	1
Caelo	Pé-de-leão	27011401	1
Caelo	Pé-de-leão	14066002	2
Caelo	Pé-de-leão	14066008	1
Caelo	Pé-de-leão	15147002	2
Caelo	Pé-de-leão	1118206	1
Caelo	Pé-de-leão	1213309	1
Caelo	Pé-de-leão	1215305	2
Caelo	Pé-de-leão	131411002	1
Caelo	Pé-de-leão	13141102	6
Caelo	Pé-de-leão	5013I1616	1
Caelo	Pé-de-leão	13141101	7
Caelo	Pé-de-leão	1215309	1
Caelo	Pé-de-leão	13141103-3382319003	1
Caelo	Pé-de-leão	13141103-3400310161	1
Caelo	Pé-de-leão	13141103-3456311103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Pé-de-leão	13141106-3545412081	1
Galke	Pé-de-leão	21141	1
Galke	Pé-de-leão	22291	1
Galke	Pé-de-leão	19835	1
Gehe	Pé-de-leão	1341102	1
Klenk	Pé-de-leão	3501C121105	4
Hepart AG	Pé-de-leão	21963	3
Hepart AG	Pé-de-leão	B-698kbA	1
Ichtyol/Phönix	Pé-de-leão	13141107	3
Klenk	Pé-de-leão	3501B100428	1
Klenk	Pé-de-leão	3501B090417	1
Klenk	Pé-de-leão	3501A110301	3
Noweda	Pé-de-leão	12153302	13
Caelo	Pé-de-leão	14066003	1
Sanacorp	Pé-de-leão	12153309	14
Caelo	Pé-de-leão	12153306	5
Fagron	Pé-de-leão	11182802	1
Wolf	Pé-de-leão	E-822	1
Wolf	Pé-de-leão	B-698	2
Wolf	Pé-de-leão	23187	4
Wolf	Pé-de-leão	p931	1
Caelo	Perborato de sódio, hidratado	13050801	2
Caelo	Perborato de sódio, hidratado	13050807	1
Caelo	Perborato de sódio, hidratado	13050805	1
Caelo	Pétala de papoula, cortada	12330205	1
Klenk	Pétala de rosa vermelha	1561A110404	1
Caelo	Pétala de rosa vermelha	10306514	1
Caelo	Pétala de rosa vermelha	11304901	3
Caelo	Pétala de rosa vermelha	11304906	1
Caelo	Pétala de rosa vermelha	11304904	4
Caelo	Pétala de rosa vermelha	11011301	1
Caelo	Pétala de rosa vermelha	12380001	4
Caelo	Pétala de rosa vermelha	11304912	2
Caelo	Pétala de rosa vermelha	12380008	1
Caelo	Pétala de rosa vermelha	13194403	4
Caelo	Pétala de rosa vermelha	10113211	1
Caelo	Pétala de rosa vermelha	12380007-3357319071	1
Caelo	Pétala de rosa vermelha	12380004	2
Caelo	Pétala de rosa vermelha	13194402	1
Klenk	Pétala de rosa vermelha	1561B101210	2
Klenk	Pétala de rosa vermelha	1561A121016-34023101	1
kräuter schulte	Pétala de rosa vermelha	47543	1
Richter	Pétala de rosa vermelha	P236157	1
Caelo	Pilosella piloselloides, cortada	3611b111005	1
Klenk	Pilosella piloselloides, cortada	B111005	1
Klenk	Pilosella piloselloides, cortada	3611B11105	1
Caelo	Pimenta	11193911	1
Caelo	Pimenta	12192304	1
Caelo	Pimenta	12192306	1
Caelo	Pimenta	12192305	1
Caelo	Pimenta	12192309	1
Caelo	Pimenta	15395310	1
Caelo	Pimenta	13221110	1
Klenk	Pimenta	A130415	2
PHOENIX 19.05.2014	Pimenta	13221105	1
Caelo	Pimenta caiena, pulverizada…	13205106	1
Caelo	Pimpinela	8111203	1
Caelo	Pimpinela	12027411	3
Caelo	Pimpinela	12027405	2
Caelo	Pimpinela	12027403	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Pimpinela	12027413	1
Caelo	Pimpinela	12027409	1
Caelo	Pimpinela	12027410	3
Caelo	Plantago (Plantago lanceolata)	13113007	6
Bahnhof-Apotheke	Plantago (Plantago lanceolata)	7-121011	1
Bombastus	Plantago (Plantago lanceolata)	276453	1
Bombastus	Plantago (Plantago lanceolata)	275479	1
Caelo	Plantago (Plantago lanceolata)	13113008	5
Caelo	Plantago (Plantago lanceolata)	23121304	1
Caelo	Plantago (Plantago lanceolata)	10315707	2
Caelo	Plantago (Plantago lanceolata)	8061208	1
Caelo	Plantago (Plantago lanceolata)	17071201	1
Caelo	Plantago (Plantago lanceolata)	10315715	9
Caelo	Plantago (Plantago lanceolata)	10315712	2
Caelo	Plantago (Plantago lanceolata)	15101204	1
Caelo	Plantago (Plantago lanceolata)	10315711	4
Caelo	Plantago (Plantago lanceolata)	20111208	1
Caelo	Plantago (Plantago lanceolata)	12225802	5
Caelo	Plantago (Plantago lanceolata)	19121202	1
Caelo	Plantago (Plantago lanceolata)	12225804	1
Caelo	Plantago (Plantago lanceolata)	12362902	7
Caelo	Plantago (Plantago lanceolata)	22021302	1
Caelo	Plantago (Plantago lanceolata)	2031302	1
Caelo	Plantago (Plantago lanceolata)	12362906	7
Caelo	Plantago (Plantago lanceolata)	25041301	1
Caelo	Plantago (Plantago lanceolata)	13113001	8
Caelo	Plantago (Plantago lanceolata)	11061304	1
Caelo	Plantago (Plantago lanceolata)	28061301	1
Caelo	Plantago (Plantago lanceolata)	25091305	1
Caelo	Plantago (Plantago lanceolata)	1362903	1
Caelo	Plantago (Plantago lanceolata)	16101304	1
Caelo	Plantago (Plantago lanceolata)	13113005	5
Caelo	Plantago (Plantago lanceolata)	15111302	1
Caelo	Plantago (Plantago lanceolata)	20111304	1
Caelo	Plantago (Plantago lanceolata)	10011402	1
Caelo	Plantago (Plantago lanceolata)	13113010	4
Caelo	Plantago (Plantago lanceolata)	4021411	1
Caelo	Plantago (Plantago lanceolata)	13410603	3
Caelo	Plantago (Plantago lanceolata)	13410601	1
Caelo	Plantago (Plantago lanceolata)	13410612	1
Caelo	Plantago (Plantago lanceolata)	14199202	1
Caelo	Plantago (Plantago lanceolata)	15096301	1
Caelo	Plantago (Plantago lanceolata)	15096308	1
Caelo	Plantago (Plantago lanceolata)	13232401	1
Caelo	Plantago (Plantago lanceolata)	10315705	1
Caelo	Plantago (Plantago lanceolata)	1313007	1
Caelo	Plantago (Plantago lanceolata)	10315714	2
Caelo	Plantago (Plantago lanceolata)	10328702	2
Caelo	Plantago (Plantago lanceolata)	12225803	2
Caelo	Plantago (Plantago lanceolata)	12362903-3388311070	1
Caelo	Plantago (Plantago lanceolata)	13113004-3488312172	1
Caelo	Plantago (Plantago lanceolata)	13113006	6
Caesar & Loretz Gm…	Plantago (Plantago lanceolata)	12362903	33
Caesar & Loretz Gm…	Plantago (Plantago lanceolata)	13113004	13
Cealo	Plantago (Plantago lanceolata)	12362907	2
Galke	Plantago (Plantago lanceolata)	20259	1
Galke	Plantago (Plantago lanceolata)	21598	1
Gehe	Plantago (Plantago lanceolata)	1080413	1
Hepart AG	Plantago (Plantago lanceolata)	20832	5
Klenk	Plantago (Plantago lanceolata)	4271A130115	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Plantago (Plantago lanceolata)	4271A-110816	1
Klenk	Plantago (Plantago lanceolata)	A110816	1
Klenk	Plantago (Plantago lanceolata)	4271A130716	1
Klenk	Plantago (Plantago lanceolata)	4281N111121	1
Klenk	Plantago (Plantago lanceolata)	4271A111125	2
Klenk	Plantago (Plantago lanceolata)	4271A100615	2
Klenk	Plantago (Plantago lanceolata)	4271A110816	2
Klenk	Plantago (Plantago lanceolata)	427A111125	1
Phoenix	Plantago (Plantago lanceolata)	4271A11016	1
Sanacorp	Plantago (Plantago lanceolata)	263401	1
Caelo	Plantago (Plantago lanceolata)	12362901	1
-	Polentilha	711M-01619	1
-	Polentilha	130849	1
Caelo	Polentilha	20081202	1
Caelo	Polentilha	8111204	1
Caelo	Polentilha	11016407	1
Caelo	Polentilha	11328109	13
Caelo	Polentilha	11328110	1
Caelo	Polentilha	11328105	7
Caelo	Polentilha	11328112	2
Caelo	Polentilha	11016404	1
Galke	Polentilha	12891	2
Gehe	Polentilha	11328101	1
Klenk	Polentilha	3551A110913	1
Klenk	Polentilha	H-280513-3	1
Klenk	Polentilha	A110913	2
Klenk	Polentilha	3551A130903	1
Phönix	Polentilha	11328107	7
Klenk	Polentilha	11328103	4
AHD	Polygonum aviculare	4301A150527	1
Caelo	Polygonum aviculare	4301A100126	2
Caelo	Polygonum aviculare	8111202	1
Caelo	Polygonum aviculare	12295702	3
Caelo	Polygonum aviculare	12295704	4
Caelo	Polygonum aviculare	4312M-01674	1
Caelo	Polygonum aviculare	12368904	1
Caelo	Polygonum aviculare	14079304	1
Caelo	Polygonum aviculare	12368903	1
Caelo	Polygonum aviculare	7102427	1
Caelo	Polygonum aviculare	12368906	3
Finze	Polygonum aviculare	10237202	1
Klenk	Polygonum aviculare	4301A120912	1
Klenk	Polygonum aviculare	4301A121120	4
Caelo	Polygonum aviculare	12368902	5
Aldrich	Propionato de sódio	U02796-056	1
Anzag	Psyllium, semente	11185818	1
Caelo	Psyllium, semente	4121201	1
Caelo	Psyllium, semente	4121202	1
Caelo	Psyllium, semente	9011302	1
Caelo	Psyllium, semente	10011303	1
Caelo	Psyllium, semente	413E-03369	1
Caelo	Psyllium, semente	3051302	1
Caelo	Psyllium, semente	19061308	1
Caelo	Psyllium, semente	18071301	1
Caelo	Psyllium, semente	5091319	1
Caelo	Psyllium, semente	30101302	1
Caelo	Psyllium, semente	16121302	1
Caelo	Psyllium, semente	26011401	1
Caelo	Psyllium, semente	14031408	1
Caelo	Psyllium, semente	11061405	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Psyllium, semente	4114001	1
Caelo	Psyllium, semente	12276527	1
Caelo	Psyllium, semente	23011505	1
Caelo	Psyllium, semente	14246602	3
Caelo	Psyllium, semente	142660	1
Caelo	Psyllium, semente	29061510	1
Caelo	Psyllium, semente	15081503	1
Caelo	Psyllium, semente	15121901	1
Caelo	Psyllium, semente	8041702	1
Caelo	Psyllium, semente	28111703	1
Caelo	Psyllium, semente	18061804	1
Caelo	Psyllium, semente	15249315	1
Caelo	Psyllium, semente	12252709	1
Caelo	Psyllium, semente	1227506	1
Caelo	Psyllium, semente	12276511	1
Caelo	Psyllium, semente	15249319	2
Caelo	Psyllium, semente	12276501	2
Caesar/Noweda	Psyllium, semente	12276503	1
Caesar/Noweda	Psyllium, semente	12276509	3
Caesar/Noweda	Psyllium, semente	12276516	1
Cealo	Psyllium, semente	12276502	4
Klenk	Psyllium, semente	7560A130710	1
Klenk	Psyllium, semente	7560A120828	7
Klenk	Psyllium, semente	20071302	1
Klenk	Psyllium, semente	7560A130418	2
Klenk	Psyllium, semente	7560A160229	1
Klenk	Psyllium, semente	7560A140203	1
Klenk	Psyllium, semente	7560A150420	3
Caelo	Psyllium, semente	11185811	2
Caelo	Pulmonária, cortada	11021707	1
Caelo	Pulmonária, cortada	11134203	12
Caelo	Pulmonária, cortada	4331b111205	1
Caelo	Pulmonária, cortada	13029302	25
Caelo	Pulmonária, cortada	11134205	3
Caelo	Pulmonária, cortada	11134201	1
Caelo	Pulmonária, cortada	13029306	3
Caelo	Pulmonária, cortada	11021709	2
Caelo	Pulmonária, cortada	13355801	2
Caesar & Loretz Gm…	Pulmonária, cortada	13029304	5
Fagron	Pulmonária, cortada	Nachprüfung	1
Galke	Pulmonária, cortada	19511	4
Klenk	Pulmonária, cortada	4331B111205	1
Klenk	Pulmonária, cortada	4331A120813	1
Richter	Pulmonária, cortada	P195884	1
Caelo	Pulmonária, cortada	11134202	3

Q

Supplier	Substance	Batch	Spectra
Anzag 26.10.12 2.36EUR	Quercus alba	10348616	6
Caelo	Quercus alba	11351202	5
Bahnhof-Apotheke	Quercus alba	17-121106	1
Berkel AHK	Quercus alba	13360310	1
Bombastus	Quercus alba	272704	1
Bombastus	Quercus alba	265717	1
Bombastus	Quercus alba	274392	1
Bombastus	Quercus alba	274611	1
Bombastus	Quercus alba	279525	2
Bombastus	Quercus alba	229090	1
Bombastus	Quercus alba	286297	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Quercus alba	15314908	2
Caelo	Quercus alba	10348612	1
Caelo	Quercus alba	22081204	1
Caelo	Quercus alba	10348615	1
Caelo	Quercus alba	7021302	1
Caelo	Quercus alba	19032013	2
Caelo	Quercus alba	3041301	1
Caelo	Quercus alba	11351201	3
Caelo	Quercus alba	11351203	1
Caelo	Quercus alba	10238612	1
Caelo	Quercus alba	16081305	1
Caelo	Quercus alba	26081302	1
Caelo	Quercus alba	5091302	1
Caelo	Quercus alba	14111316	1
Caelo	Quercus alba	161212	1
Caelo	Quercus alba	41109-4-P	1
Caelo	Quercus alba	1135121o	1
Caelo	Quercus alba	123test	1
Caelo	Quercus alba	13360301	1
Caelo	Quercus alba	1081401	1
Caelo	Quercus alba	280814A	1
Caelo	Quercus alba	13360304	1
Caelo	Quercus alba	13360311	1
Caelo	Quercus alba	13360309	1
Caelo	Quercus alba	10061504	1
Caelo	Quercus alba	14277004	1
Caelo	Quercus alba	14277004	2
Caelo	Quercus alba	15146104	4
Caelo	Quercus alba	15146103	1
Caelo	Quercus alba	15146105	4
Caelo	Quercus alba	15146110	1
Caelo	Quercus alba	15146110	1
Caelo	Quercus alba	15314904	1
Caelo	Quercus alba	15314904	4
Caelo	Quercus alba	15314906	1
Caelo	Quercus alba	15314912	3
Caelo	Quercus alba	501919	1
Caelo	Quercus alba	18014702	1
Caelo	Quercus alba	19133902	1
Caelo	Quercus alba	18014701	1
Caelo	Quercus alba	15314903	1
Caelo	Quercus alba	15146109	2
Caelo	Quercus alba	10348613	2
Caelo	Quercus alba	11351210	8
Caelo	Quercus alba	11351207-3384310110	1
Caelo	Quercus alba	13360305	1
Caelo	Quercus alba	13360308	1
Caelo	Quercus alba	14277004	1
Caelo	Quercus alba	15146105	1
Caelo	Quercus alba	15314910	6
Caelo	Quercus alba	13360306	2
Caelo	Quercus alba	13360312	5
Caelo	Quercus alba	15146101	2
Caelo	Quercus alba	15146102	1
Caelo	Quercus alba	10348605	1
Caelo	Quercus alba	16305701	1
Caelo	Quercus alba	15314901	1
Caelo	Quercus alba	15314911	1
Caelo	Quercus alba	12221102	1
Caelo	Quercus alba	9357419	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Quercus alba	12221101	9
Caelo	Quercus alba	13360303	1
Caelo	Quercus alba	13360306	1
Caelo	Quercus alba	15314905	3
Caelo	Quercus alba	12221104	2
Caelo	Quercus alba	11351205	3
Caelo	Quercus alba	11351208	3
Euro OTC	Quercus alba		1
Galke	Quercus alba	17824	2
GEHE 10.03.2014	Quercus alba	761A11816	1
Gutenberg-Apotheke	Quercus alba	11351206	13
Caelo	Quercus alba	11351209	10
Klenk	Quercus alba	C-280513-2	1
Klenk	Quercus alba	761A110816	1
Klenk	Quercus alba	761A090420	1
Klenk	Quercus alba	761A110816	10
Noweda	Quercus alba	10348617	8
Caelo	Quercus alba	11351207	11
Klenk	Quercus alba	761A110816	1
Caelo	Quercus alba	12221105	2
Caelo	Quercus alba	13360302	6
Phönix	Quercus alba	10348609	2

R

Supplier	Substance	Batch	Spectra
Caelo	Raiz de aipo, cortada	12319105	2
Caelo	Raiz de aipo, cortada	12319107	1
Caelo	Raiz de aipo, cortada	10270009	1
Caelo	Raiz de aipo, cortada	10270012	1
Caelo	Raiz de aipo, cortada	12319108	1
Klenk	Raiz de aipo, cortada	6091A110110	1
aurica/phoenix	Raiz de alcaçuz	521206925	1
Bombastus	Raiz de alcaçuz	2901312151	1
Bombastus	Raiz de alcaçuz	903312151	1
Bombastus	Raiz de alcaçuz	279409	2
Bombastus	Raiz de alcaçuz	5091305	1
Bombastus	Raiz de alcaçuz	285185	2
Bombastus	Raiz de alcaçuz	286584	1
Bombastus	Raiz de alcaçuz	278377	3
Bombastus	Raiz de alcaçuz	274921	3
Bombastus	Raiz de alcaçuz	3713Q2151	1
Caelo	Raiz de alcaçuz	13037904	1
Caelo	Raiz de alcaçuz	10110912	1
Caelo	Raiz de alcaçuz	12267103	1
Caelo	Raiz de alcaçuz	13037902	1
Caelo	Raiz de alcaçuz		1
Caelo	Raiz de alcaçuz	12267104	2
Gehe	Raiz de alcaçuz	277004	2
Gehe	Raiz de alcaçuz	283316	1
Gehe	Raiz de alcaçuz	284243	2
Klenk	Raiz de alcaçuz	6391A080905	4
Klenk	Raiz de alcaçuz	6391A110421	4
Klenk	Raiz de alcaçuz	6390A101020	1
PHOENIX am 27.12.2013	Raiz de alcaçuz	281844	1
Bombastus	Raiz de alcaçuz	276468	6
Phönix	Raiz de alcaçuz	276425	1
Bahnhof-Apotheke	Raiz de alcaçuz, descascada	17-121112	1
Bombastus	Raiz de alcaçuz, descascada	268001	1
Bombastus	Raiz de alcaçuz, descascada	270192	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Raiz de alcaçuz, descascada	6381A111004	14
Caelo	Raiz de alcaçuz, descascada	1135904	1
Caelo	Raiz de alcaçuz, descascada	11351911	4
Caelo	Raiz de alcaçuz, descascada	10011301	1
Caelo	Raiz de alcaçuz, descascada	1351911	1
Caelo	Raiz de alcaçuz, descascada	11351913	1
Caelo	Raiz de alcaçuz, descascada	11351910	2
Caelo	Raiz de alcaçuz, descascada	638a120806	1
Caelo	Raiz de alcaçuz, descascada	13104503	3
Caelo	Raiz de alcaçuz, descascada	13104504	4
Caelo	Raiz de alcaçuz, descascada	18121302	1
Caelo	Raiz de alcaçuz, descascada	13194101	5
Caesar & Loretz Gm...	Raiz de alcaçuz, descascada	11034014	1
Galke	Raiz de alcaçuz, descascada	23538	1
Gehe	Raiz de alcaçuz, descascada	268835	1
Gehe	Raiz de alcaçuz, descascada	270853	3
Gehe	Raiz de alcaçuz, descascada	1250213	1
Caelo	Raiz de alcaçuz, descascada	12227112	1
Klenk	Raiz de alcaçuz, descascada	6381a111004	1
Klenk	Raiz de alcaçuz, descascada	6381A121126	27
Klenk	Raiz de alcaçuz, descascada	6381A130426	21
Klenk	Raiz de alcaçuz, descascada	A130426	1
Klenk	Raiz de alcaçuz, descascada	A130820	3
Klenk	Raiz de alcaçuz, descascada	6381A130820	4
Klenk	Raiz de alcaçuz, descascada	6381A140109	2
Klenk	Raiz de alcaçuz, descascada	6381A130425	1
Klenk	Raiz de alcaçuz, descascada	6381A110531	2
Klenk	Raiz de alcaçuz, descascada	638A130820	1
Klenk	Raiz de alcaçuz, descascada	6381a121126	1
Noweda	Raiz de alcaçuz, descascada	70226/1	1
Klenk	Raiz de alcaçuz, descascada	6381A120806	3
Phoenix	Raiz de alcaçuz, descascada	6381A120611	12
Sanacorp	Raiz de alcaçuz, descascada	11351906	3
Caelo	Raiz de alcaçuz, descascada	277004	1
Caelo	Raiz de alcaçuz, descascada	11351905	3
-	Raiz de angélica	130924	1
Bombastus	Raiz de angélica	275879	1
Aurica/Phönix	Raiz de angélica	520800638	1
Bombastus	Raiz de angélica	272895	1
Bombastus	Raiz de angélica	274128	2
Bombastus	Raiz de angélica	269775	2
Bombastus	Raiz de angélica	272954	1
Bombastus	Raiz de angélica	270117	1
Bombastus	Raiz de angélica	281280	7
Bombastus	Raiz de angélica	301768	1
Bombastus	Raiz de angélica	290309	1
Bombastus	Raiz de angélica	307041	4
Bombastus	Raiz de angélica	291848	1
Bombastus	Raiz de angélica	295085	2
Bombastus	Raiz de angélica	305460	1
Bombastus	Raiz de angélica	275878	1
Caelo	Raiz de angélica	11093304	1
Caelo	Raiz de angélica	12168703	2
Caelo	Raiz de angélica	12080403	1
Caelo	Raiz de angélica	30011302	1
Caelo	Raiz de angélica	269740	1
Caelo	Raiz de angélica	6081B130109	7
Caelo	Raiz de angélica	10071306	1
Caelo	Raiz de angélica	Int.Ch:318090	1
Caelo	Raiz de angélica	12350705	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Raiz de angélica	5091303	1
Caelo	Raiz de angélica	15101304	1
Caelo	Raiz de angélica	21011402	1
Caelo	Raiz de angélica	12080412	1
Caelo	Raiz de angélica	28101402	1
Caelo	Raiz de angélica	13041711	1
Caelo	Raiz de angélica	17053302	1
Caelo	Raiz de angélica	12168701	3
Caelo	Raiz de angélica	12350703	9
Caelo	Raiz de angélica	12350704	2
Caelo	Raiz de angélica	15162604	2
Caelo	Raiz de angélica	12168705	2
Caelo	Raiz de angélica	14179506	2
Caelo	Raiz de angélica	16128006	1
Caelo	Raiz de angélica	285732	2
Caelo	Raiz de angélica	16128002	3
Caelo	Raiz de angélica	9030301	1
Caelo	Raiz de angélica	303299	1
Caelo	Raiz de angélica	5162606	1
Caelo	Raiz de angélica	17053301	1
Euro OTC	Raiz de angélica	301767	3
gasser	Raiz de angélica	950049	1
Gehe	Raiz de angélica	285732	1
Bombastus	Raiz de angélica	296334/1121115	1
Klenk	Raiz de angélica	6081B130410	4
Klenk	Raiz de angélica	17053308	1
Klenk	Raiz de angélica	6081N120110	14
Klenk	Raiz de angélica	6081n120110	1
Klenk	Raiz de angélica	B130109	2
Klenk	Raiz de angélica	6091B130109	1
Klenk	Raiz de angélica	6081B130109	1
Klenk	Raiz de angélica	6081B140918	2
Klenk	Raiz de angélica	6081B130726	1
Klenk	Raiz de angélica	6081B150701	7
Klenk	Raiz de angélica		1
Klenk	Raiz de angélica	6081B170601	4
Klenk	Raiz de angélica	6085B120614	1
Klenk	Raiz de angélica	6081b130109	2
Klenk	Raiz de angélica	6082b130410	1
Caelo	Raiz de angélica	17053304	2
Noweda	Raiz de angélica	272720	2
Bombastus	Raiz de angélica	278294	1
Bombastus	Raiz de angélica	278757	4
Caelo	Raiz de angélica	14178506	1
Sanacorp	Raiz de angélica	277310	1
Klenk	Raiz de angélica	6081B160908	1
Weltecke	Raiz de angélica	38011111	1
Caelo	Raiz de aspargo, cortada	13193302	1
Caelo	Raiz de aspargo, cortada	13193308	1
Caelo	Raiz de aspargo, cortada	15010802	1
Galke	Raiz de aspargo, cortada	20178	1
Caelo	Raiz de aspargo, cortada	13071002	1
Klenk	Raiz de aspargo, cortada	6151B100332	1
Caelo	Raiz de Astrantia major, cortada	1210801	1
Caelo	Raiz de Astrantia major, cortada	12101806	2
Caelo	Raiz de Astrantia major, cortada	12101808	1
Caelo	Raiz de Astrantia major, cortada	13132002	1
Caelo	Raiz de Astrantia major, cortada	13341201	1
Caelo	Raiz de Astrantia major, cortada	12101807	2
Galke	Raiz de Astrantia major, cortada	18411	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Galke	Raiz de Astrantia major, cortada	23074	1
-	Raiz de bardana	5110I-02131	1
Caelo	Raiz de bardana	12295808	2
Caelo	Raiz de bardana	12295801	2
Caelo	Raiz de bardana	1100801	1
Caelo	Raiz de bardana	10073213	1
Caelo	Raiz de bardana	11100801	2
Caelo	Raiz de bardana	12295805	3
Caelo	Raiz de bardana	12295807	1
Caelo	Raiz de bardana	13122802	1
Caelo	Raiz de bardana	13122801	2
Caelo	Raiz de bardana	12295802	4
Caelo	Raiz de bardana	107063	1
Euro OTC	Raiz de bardana	13122803	1
Galke	Raiz de bardana	19802	1
Klenk	Raiz de bardana	6161A101206	1
Klenk	Raiz de bardana	6161A120208	4
Klenk	Raiz de bardana	A120206	1
Klenk	Raiz de bardana	A130214	1
Klenk	Raiz de bardana	6161A080709	1
Klenk	Raiz de bardana	6161A-101206	1
Klenk	Raiz de bardana	6161A120103	1
Klenk	Raiz de bardana	6161A-120103	1
Bombastus	Raiz de cálamo	276260	2
Bombastus	Raiz de cálamo	224114	1
Bombastus	Raiz de cálamo	281692	2
Bombastus	Raiz de cálamo	277958	1
Bombastus	Raiz de cálamo	274159	1
Caelo	Raiz de cálamo	13127801	1
Caelo	Raiz de cálamo	284875	2
Klenk	Raiz de cálamo	B130807	1
Caelo	Raiz de cálamo	12066501	1
Aurica/Phönix	Raiz de cálamo, descascada	150649	1
Bahnhof-Apotheke	Raiz de cálamo, descascada	17-121107	1
Bombastus	Raiz de cálamo, descascada	267365	1
Bombastus	Raiz de cálamo, descascada	274159	3
Caelo	Raiz de cálamo, descascada	15061202	1
Caelo	Raiz de cálamo, descascada	24081203	1
Caelo	Raiz de cálamo, descascada	12056703	1
Caelo	Raiz de cálamo, descascada	12066501	7
Caelo	Raiz de cálamo, descascada	12066502	1
Caelo	Raiz de cálamo, descascada	28121205	1
Caelo	Raiz de cálamo, descascada	8031306	1
Caelo	Raiz de cálamo, descascada	12295901	1
Caelo	Raiz de cálamo, descascada	6701B130103	21
Caelo	Raiz de cálamo, descascada	12295904	4
Caelo	Raiz de cálamo, descascada	7061302	1
Caelo	Raiz de cálamo, descascada	313060	1
Caelo	Raiz de cálamo, descascada	12295903	1
Caelo	Raiz de cálamo, descascada	12275602	7
Caelo	Raiz de cálamo, descascada	241013010	1
Caelo	Raiz de cálamo, descascada	12275604	2
Caelo	Raiz de cálamo, descascada	12056701	1
Caelo	Raiz de cálamo, descascada	12295902	4
Caelo	Raiz de cálamo, descascada	12239008	1
Caelo	Raiz de cálamo, descascada	12275604-3544411013	1
Caelo	Raiz de cálamo, descascada	13101306	1
Galke	Raiz de cálamo, descascada	18944	1
Gehe	Raiz de cálamo, descascada	6701B130807	9
Klenk	Raiz de cálamo, descascada	6701B150407	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Raiz de cálamo, descascada	106212173	1
Klenk	Raiz de cálamo, descascada	6701B120427	7
Klenk	Raiz de cálamo, descascada	6701B120817	6
Klenk	Raiz de cálamo, descascada	6701B130870	1
Klenk	Raiz de cálamo, descascada	6711B110606	1
Klenk	Raiz de cálamo, descascada	4797362	1
Klenk	Raiz de cálamo, descascada	6701b120301	1
Klenk	Raiz de cálamo, descascada	6701b130103	1
Klenk	Raiz de cálamo, descascada	6701B120301	3
Caelo	Raiz de Carlina acaulis	23071203	1
Caelo	Raiz de Carlina acaulis	12144804	1
Caelo	Raiz de Carlina acaulis	13130303	1
Caelo	Raiz de Carlina acaulis	13033501	1
Caelo	Raiz de Carlina acaulis	25111306	1
Caelo	Raiz de Carlina acaulis	14347401	1
Caelo	Raiz de Carlina acaulis	13130301	6
Caelo	Raiz de Carlina acaulis	13130304	1
Caelo	Raiz de Carlina acaulis	12232803	1
Hepart AG	Raiz de Carlina acaulis	B120726	1
Klenk	Raiz de Carlina acaulis	12097301	1
Klenk	Raiz de Carlina acaulis	B110831	1
Klenk	Raiz de Carlina acaulis	6194b110831	1
Klenk	Raiz de Carlina acaulis	6194B110831	1
Klenk	Raiz de Carlina acaulis	6191B120726	3
Klenk	Raiz de Carlina acaulis	69191B120726	1
Nachprüfung	Raiz de Carlina acaulis	2812U02133	1
Noweda	Raiz de Carlina acaulis	12163702	1
Caelo	Raiz de confrei	2711Q-02135	1
Caelo	Raiz de confrei	116053	1
Hof-Apotheke,St.Afra	Raiz de confrei	125041	1
Klenk	Raiz de confrei	6241B120531	3
Klenk	Raiz de confrei	6241B120807	4
Klenk	Raiz de confrei	6241B100715	1
Klenk	Raiz de confrei	6241B130619	8
Klenk	Raiz de confrei	B130619	1
Klenk	Raiz de confrei	6241B130724	7
Klenk	Raiz de confrei	6241B131009	1
Klenk	Raiz de confrei	6241B121214	2
Klenk	Raiz de confrei	6244B130624	1
Klenk	Raiz de confrei	6241B06110202	1
Klenk	Raiz de confrei	6241B130312	3
Klenk	Raiz de confrei	6241b130619	1
Klenk	Raiz de confrei	6241b130724	1
Klenk	Raiz de confrei	6241b120807	1
-	Raiz de elecampane, cortada	712M-02181	1
Caelo	Raiz de elecampane, cortada	12113304	3
Caelo	Raiz de elecampane, cortada	1211334	1
Caelo	Raiz de elecampane, cortada	6341B	1
Caelo	Raiz de elecampane, cortada	11374702	1
Caelo	Raiz de elecampane, cortada	13152402	1
Caelo	Raiz de elecampane, cortada	13152401	1
Caelo	Raiz de elecampane, cortada	12113303	1
Galke	Raiz de elecampane, cortada	21569	2
Gehe	Raiz de elecampane, cortada	11196906	1
Gehe	Raiz de elecampane, cortada	12113302	2
Caelo	Raiz de elecampane, cortada	11374703	1
Klenk	Raiz de elecampane, cortada	6341B100426	2
Klenk	Raiz de elecampane, cortada	6341B120611	2
Klenk	Raiz de elecampane, cortada	B130423	3
Klenk	Raiz de elecampane, cortada	6341B130423	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Raiz de elecampane, cortada	6311141B130423	1
Noweda	Raiz de elecampane, cortada	6341B111118	3
Caelo	Raiz de elecampane, cortada	13152403	2
Richter	Raiz de elecampane, cortada	P158683	1
Klenk	Raiz de fraxinela, cortada	6271B140708	1
Caelo	Raiz de garra-do-diabo	12031806	1
Caelo	Raiz de garra-do-diabo	12031810	1
Caelo	Raiz de garra-do-diabo	12031809	1
Caelo	Raiz de garra-do-diabo	12031811	1
Caelo	Raiz de garra-do-diabo	6331B110426	2
Caelo	Raiz de garra-do-diabo	12031803	1
Galke	Raiz de garra-do-diabo	20282	2
Galke	Raiz de garra-do-diabo	21018	2
Gehe	Raiz de garra-do-diabo	1114005	1
Klenk	Raiz de garra-do-diabo	10111204	1
Klenk	Raiz de garra-do-diabo	6331B130129	5
Klenk	Raiz de garra-do-diabo	6331B120508	3
an	Raiz de genciana	6311b130305	1
Anzag EK7,91 08.08.12	Raiz de genciana	10263407	1
Caelo	Raiz de genciana	10263404	1
Caelo	Raiz de genciana	10263411	1
Caelo	Raiz de genciana	30011301	1
Caelo	Raiz de genciana	19071304	1
Caelo	Raiz de genciana	Int.Ch:313091	1
Caelo	Raiz de genciana	12244608	1
Caelo	Raiz de genciana	6311B130305	2
Caelo	Raiz de genciana	13156102	1
Caelo	Raiz de genciana	12244607	1
Caesar & Loretz Gm...	Raiz de genciana	12244603	2
Galke	Raiz de genciana	19192	2
Klenk	Raiz de genciana	6311B130205	2
Klenk	Raiz de genciana	6311B140704	1
Klenk	Raiz de genciana	6311A120723	3
Klenk	Raiz de genciana	6311a120723	2
Klenk	Raiz de genciana	1911E-02142	1
kräuter schulte	Raiz de genciana	52348	1
Phoenix	Raiz de genciana	6311B120104	1
Phönix	Raiz de genciana	269197	2
Phönix	Raiz de genciana	6311B120315	8
Richter	Raiz de genciana	P200907	1
-	Raiz de genciana, pulverizada	130063	1
Caelo	Raiz de genciana, pulverizada	15011403	1
Caelo	Raiz de genciana, pulverizada	14215601	1
Caelo	Raiz de genciana, pulverizada	12007106	1
Bombastus	Raiz de ginseng	13150903	1
Caelo	Raiz de ginseng	13341001	1
Caelo	Raiz de ginseng	12080218	1
Bombastus	Raiz de marshmallow	273458	1
Caelo	Raiz de marshmallow	26091201	1
Caelo	Raiz de marshmallow	11101907	7
Caelo	Raiz de marshmallow	11101804	1
Caelo	Raiz de marshmallow	6071A130116	10
Caelo	Raiz de marshmallow	12147311	1
Caelo	Raiz de marshmallow	12147311	7
Caelo	Raiz de marshmallow	13057103	1
Caelo	Raiz de marshmallow	12368906	1
Caelo	Raiz de marshmallow	15104503	1
Caelo	Raiz de marshmallow	11101905	1
Caelo	Raiz de marshmallow	11101804	1
Gehe	Raiz de marshmallow	6071A120306	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Raiz de marshmallow	6071A130612	4
Klenk	Raiz de marshmallow	6074B100416	1
Klenk	Raiz de marshmallow	6071A120314	10
Klenk	Raiz de marshmallow	6071A-130408	1
Klenk	Raiz de marshmallow	A130408	3
Klenk	Raiz de marshmallow	6071A-120314	1
Klenk	Raiz de marshmallow	130116	1
Klenk	Raiz de marshmallow	6071a130408	1
Klenk	Raiz de marshmallow	6071B091207	1
Phönix	Raiz de marshmallow	6071a120314	1
Phönix	Raiz de marshmallow	2090413	1
Phönix	Raiz de marshmallow	6071A130408	14
Bombastus	Raiz de marshmallow, natural	270467	1
Bombastus	Raiz de marshmallow, natural	276741	1
Caelo	Raiz de marshmallow, natural	270114	1
Caelo	Raiz de Ononis repens	71035467	1
Bombastus	Raiz de Ononis repens	274421	1
Bombastus	Raiz de Ononis repens	272831	2
Bombastus	Raiz de Ononis repens	283708	1
Caelo	Raiz de Ononis repens	11247302	2
Caelo	Raiz de Ononis repens	11103105	2
Caelo	Raiz de Ononis repens	6101201	1
Caelo	Raiz de Ononis repens	20111213	1
Caelo	Raiz de Ononis repens	21011306	1
Caelo	Raiz de Ononis repens	12330001	14
Caelo	Raiz de Ononis repens	1233001	2
Caelo	Raiz de Ononis repens	Int.Ch:212150	1
Caelo	Raiz de Ononis repens	12330005	5
Caelo	Raiz de Ononis repens	15101313	1
Caelo	Raiz de Ononis repens	4021406	1
Caelo	Raiz de Ononis repens	12330002	1
Caelo	Raiz de Ononis repens	12330003	2
Caelo	Raiz de Ononis repens	1230004	1
Caelo	Raiz de Ononis repens	72439069	1
Caesar/Noweda	Raiz de Ononis repens	71015/3	2
Galke	Raiz de Ononis repens	12700	1
Hepart AG	Raiz de Ononis repens	B130404	3
Klenk	Raiz de Ononis repens	6411111110	1
Klenk	Raiz de Ononis repens	6411B101216	2
Klenk	Raiz de Ononis repens	4296345	1
Klenk	Raiz de Ononis repens	6411B111110	1
Klenk	Raiz de Ononis repens	B111110	1
Klenk	Raiz de Ononis repens	6411B130404	2
Caelo	Raiz de Ononis repens	11103107	2
Caelo	Raiz de Orris	11026704	2
Caelo	Raiz de Orris	11026706	1
Caelo	Raiz de Orris	13113401	2
Caelo	Raiz de Orris	1026706	1
Caelo	Raiz de Orris	13113404	1
Fagron	Raiz de Orris	11026705	3
Galke	Raiz de Orris	21303	1
Klenk	Raiz de Orris	B111013	1
Klenk	Raiz de Orris	6831B111013	1
Klenk	Raiz de Orris	B130102	1
Sanacorp	Raiz de Orris	11026701	1
Caelo	Raiz de Orris	13113402	1
Klenk	Raiz de peônia, cortada	B110916	2
Klenk	Raiz de peônia, cortada	6421B120327	1
Caelo	Raiz de prímula, cortada	13087005	3
Caelo	Raiz de prímula, cortada	10382009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Raiz de prímula, cortada	10382013	1
Caelo	Raiz de prímula, cortada	12064503	1
Caelo	Raiz de prímula, cortada	10382012	1
Caelo	Raiz de prímula, cortada	12064506	4
Caelo	Raiz de prímula, cortada	24011301	1
Caelo	Raiz de prímula, cortada	5010E-02159	1
Caelo	Raiz de prímula, cortada	Int.Ch:318090	1
Caelo	Raiz de prímula, cortada	13087004	1
Caelo	Raiz de prímula, cortada	4021410	1
Caelo	Raiz de prímula, cortada	10382010	1
Caelo	Raiz de prímula, cortada	13067001	1
Caelo	Raiz de prímula, cortada	13087001	1
Caelo	Raiz de prímula, cortada	71653517	1
Caelo	Raiz de prímula, cortada	13087005-3534411072	1
Caelo	Raiz de prímula, cortada	13087002	4
Klenk	Raiz de prímula, cortada	6461A100511	1
Klenk	Raiz de prímula, cortada	B130218	3
Noweda	Raiz de prímula, cortada	12064504	4
Klenk	Raiz de sabugueiro, cortada	6281B110427	4
Probe	Raiz de sabugueiro, cortada	12345	1
Caelo	Raiz de salsa	12080309	1
Caelo	Raiz de salsa	12080304	1
Caelo	Raiz de salsa	13156003	1
Caelo	Raiz de salsa	13156005	1
Gahlke	Raiz de salsa	20872	1
Gehe	Raiz de salsa	6441A110210	3
Klenk	Raiz de salsa	6441A150811	1
Klenk	Raiz de salsa	6441A120606	5
Klenk	Raiz de salsa	6441A121024	4
Klenk	Raiz de salsa	6441A120283	1
Kräuter Schulte	Raiz de saponária, cortada	54524	2
Kräuter Schulte	Raiz de saponária, cortada	54977	1
Kräuter Schulte	Raiz de saponária, cortada	54500	1
Berkel AHK	Raiz de valeriana, pulverizada	13287406	1
Berkel AHK	Raiz de valeriana, pulverizada	14179403	2
Caelo	Raiz de valeriana, pulverizada	13287402	2
Caelo	Raiz de valeriana, pulverizada	15175204	1
Caelo	Raiz de zedoária	11091603	1
Caelo	Raiz de zedoária	13010104	1
Caelo	Raiz de zedoária	25111304	1
Caelo	Raiz de zedoária	12125301	3
Caelo	Raiz de zedoária	13010102	3
Caelo	Raiz de zedoária	12125304	2
Klenk	Raiz de zedoária	6941B121025	3
Klenk	Raiz de zedoária	6941B110329	2
Noweda	Raiz de zedoária	11091605	3
Caelo	Raiz de zedoária	111091607	1
vedono	Raiz de zedoária	13010106	3
Caelo	Raiz de zedoária, pulverizada	12007504	1
Caelo	Raiz de zedoária, pulverizada	13165501	2
Caelo	Raiz de zedoária, pulverizada	13165504	4
Caelo	Raiz de zedoária, pulverizada	15277101	1
Caelo	Raiz de zedoária, pulverizada	15352606	1
Klenk	Raiz de zedoária, pulverizada	12007505	1
Caelo	Resina Podophyllum (de Podo…	11085807	4
Caelo	Resina Podophyllum (de Podo…	12287805	1
Caelo	Resina Podophyllum (de Podo…	11085811	1
Caelo	Resina Podophyllum (de Podo…	12379903	1
Caelo	Resina Podophyllum (de Podo…	12287810	1
Caelo	Resina Podophyllum (de Podo…	82433349	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Rizoma de galanga	12330305	1
Caelo	Rizoma de galanga	11375904	1
Caelo	Rizoma de galanga	12330306	2
Caelo	Rizoma de galanga	15128008	1
Caelo	Rizoma de galanga	16196901	1
Caelo	Rizoma de galanga	4056371	1
Caelo	Rizoma de galanga	94614429	1
Caelo	Rizoma de galanga	16196904	1
Caelo	Rizoma de galanga	12125004	2
Caelo	Rizoma de galanga	1215004	1
Caelo	Rizoma de galanga	12330303	1
Caelo	Rizoma de galanga	15045701	1
Bombastus	Rizoma de grama-francesa, c...	276777	3
Bombastus	Rizoma de grama-francesa, c...	273387	3
Bombastus	Rizoma de grama-francesa, c...	270500	2
Bombastus	Rizoma de grama-francesa, c...	278926	1
Bombastus	Rizoma de grama-francesa, c...	262175	1
Caelo	Rizoma de grama-francesa, c...	10049614	1
Caelo	Rizoma de grama-francesa, c...	10049618	2
Caelo	Rizoma de grama-francesa, c...	10349705	1
Caelo	Rizoma de grama-francesa, c...	10349704	1
Caelo	Rizoma de grama-francesa, c...	3712I-02180	1
Caelo	Rizoma de grama-francesa, c...	12186817	3
Caelo	Rizoma de grama-francesa, c...	12186705	1
Caesar/Noweda	Rizoma de grama-francesa, c...	12186813	4
Galke	Rizoma de grama-francesa, c...	18781	1
Gehe	Rizoma de grama-francesa, c...	12186704	1
Gehe	Rizoma de grama-francesa, c...	283061	1
Kräuter Schulte	Rizoma de grama-francesa, c...	53016	2
Caelo	Rosa canina, casca	12064207	1
Bombastus	Rosa canina, casca	275394	2
Bombastus	Rosa canina, casca	283458	1
Bombastus	Rosa canina, casca	257166	1
Bombastus	Rosa canina, casca	277431	3
Bombastus	Rosa canina, casca	285184	1
Bombastus	Rosa canina, casca	231013A	1
Caelo	Rosa canina, casca	15061210	1
Caelo	Rosa canina, casca	25061203	1
Caelo	Rosa canina, casca	11301405	2
Caelo	Rosa canina, casca	10101206	1
Caelo	Rosa canina, casca	11301401	1
Caelo	Rosa canina, casca	7031305	1
Caelo	Rosa canina, casca	12288301	1
Caelo	Rosa canina, casca	12357501	1
Caelo	Rosa canina, casca	12357505	6
Caelo	Rosa canina, casca	5091301	1
Caelo	Rosa canina, casca	12357504	2
Caelo	Rosa canina, casca	9121301	1
Caelo	Rosa canina, casca	14050704	1
Caelo	Rosa canina, casca	14050705	1
Caelo	Rosa canina, casca	2851A120904konv.	1
Caelo	Rosa canina, casca	10157309	1
Caelo	Rosa canina, casca	13317805	1
Caelo	Rosa canina, casca	11301403	2
Caelo	Rosa canina, casca	13317801	2
Caelo	Rosa canina, casca	12357502	3
Klenk	Rosa canina, casca	2851A150310	4
Klenk	Rosa canina, casca	2851A101119	3
Klenk	Rosa canina, casca	2851A110202	1
Klenk	Rosa canina, casca	2841B111019	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Rosa canina, casca	2851A120102	5
Klenk	Rosa canina, casca	2851A120904	2
Klenk	Rosa canina, casca	A120904	3
Klenk	Rosa canina, casca	2851A-110202	1
Klenk	Rosa canina, casca	3613M-01543	1
Caelo	Rosa canina, casca	11301407	12
Caelo	Rosa canina, casca	12288302	7
Aurica	Rosa-mosqueta com casca, cortada	521201801	1
Caelo	Rosa-mosqueta com casca, cortada	307211542	1
Caelo	Rosa-mosqueta com casca, cortada	16111201	1
Caelo	Rosa-mosqueta com casca, cortada	19111204	1
Caelo	Rosa-mosqueta com casca, cortada	12064207	2
Caelo	Rosa-mosqueta com casca, cortada	1512211542	1
Caelo	Rosa-mosqueta com casca, cortada	12064210	3
Caelo	Rosa-mosqueta com casca, cortada	2103311542	1
Caelo	Rosa-mosqueta com casca, cortada	12064209	4
Caelo	Rosa-mosqueta com casca, cortada	12029011	1
Caelo	Rosa-mosqueta com casca, cortada	12064213	1
Caelo	Rosa-mosqueta com casca, cortada	13048703	1
Caelo	Rosa-mosqueta com casca, cortada	13048704	1
Caelo	Rosa-mosqueta com casca, cortada	13048704	3
Caelo	Rosa-mosqueta com casca, cortada	12029008	1
Caelo	Rosa-mosqueta com casca, cortada	12064210	2
Caelo	Rosa-mosqueta com casca, cortada	12064212	3
Caelo	Rosa-mosqueta com casca, cortada	12064201	1
Caelo	Rosa-mosqueta com casca, cortada	12064209	1
Caelo	Rosa-mosqueta com casca, cortada	12064213	1
Caelo	Rosa-mosqueta com casca, cortada	13048703	1
Caelo	Rosa-mosqueta com casca, cortada	12064202	1
Caelo	Rosa-mosqueta com casca, cortada	12064207	3
Caelo	Rosa-mosqueta com casca, cortada	13048701	2
Caelo	Rosa-mosqueta com casca, cortada	114Q-01542	1
Caelo	Rosa-mosqueta com casca, cortada	13097405	1
Caelo	Rosa-mosqueta com casca, cortada	12064212	2
Klenk	Rosa-mosqueta com casca, cortada	B111019	1
Klenk	Rosa-mosqueta com casca, cortada	A120719	1
Klenk	Rosa-mosqueta com casca, cortada	B130523	1
Klenk	Rosa-mosqueta com casca, cortada	A120904	1
Klenk	Rosa-mosqueta com casca, cortada	2841B081210	1
Klenk	Rosa-mosqueta com casca, cortada	2841B111019	3
Klenk	Rosa-mosqueta com casca, cortada	3613M-01542	1
Klenk	Rosa-mosqueta com casca, cortada	2851A120904	1
Phönix	Rosa-mosqueta com casca, cortada	10281021	1
Phönix	Rosa-mosqueta com casca, cortada	2841B130523	1
Phönix	Rosa-mosqueta com casca, cortada	2841B130523	1
Caelo	Rosa-mosqueta com casca, cortada	12064202	1
Caelo	Rosa-mosqueta com casca, cortada	12064206	1
Caelo	Ruibarbo	11265902	1
Caelo	Ruibarbo	11057810	1
Caelo	Ruibarbo	12211903	4
Caelo	Ruibarbo	11057818	2
Caelo	Ruibarbo	10071302	1
Caelo	Ruibarbo	12211908	1
Caelo	Ruibarbo	11321806	1
Caelo	Ruibarbo	15101301	1
Caelo	Ruibarbo	13235201	2
Caelo	Ruibarbo	25111305	1
Caelo	Ruibarbo	14155404	1
Caelo	Ruibarbo	12211904	2
Caelo	Ruibarbo	12211902	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ruibarbo	13235205	1
Caelo	Ruibarbo	11057804	1
Caelo	Ruibarbo	12211906	1
Caelo	Ruibarbo	13235203	1
Gehe	Ruibarbo	13235208	2
Klenk	Ruibarbo	6891B111118	1
Klenk	Ruibarbo	7761B130514	2
Phoenix	Ruibarbo	11057817	3
Phönix	Ruibarbo	12211905	3
vedono	Ruibarbo	12211907	6
Bombastus	Ruibarbo, pulverizado	11043806	1
Caelo	Ruibarbo, pulverizado	11043819	2
Caelo	Ruibarbo, pulverizado	9071201	1
Caelo	Ruibarbo, pulverizado	11043817	1
Caelo	Ruibarbo, pulverizado	11043818	1
Caelo	Ruibarbo, pulverizado	11043816	1
Caelo	Ruibarbo, pulverizado	11043826	1
Caelo	Ruibarbo, pulverizado	13193106	2
Caelo	Ruibarbo, pulverizado	23061402	1
Caelo	Ruibarbo, pulverizado	11043809	1
Caelo	Ruibarbo, pulverizado	11043816	2
Caelo	Ruibarbo, pulverizado	11043818	1
Caelo	Ruibarbo, pulverizado	11043825	2
Caelo	Ruibarbo, pulverizado	11043822	1
Caelo	Ruibarbo, pulverizado	13193104	4
Caelo	Ruibarbo, pulverizado	13193109	1
Fagron	Ruibarbo, pulverizado	11043821	1
Hedinger	Ruibarbo, pulverizado	13193110	1
Fagron	Rutosídeo tri-hidratado	13K12-B06	1
Fagron	Rutosídeo tri-hidratado	13K12-B06295483	1
Fagron	Rutosídeo tri-hidratado	13K12B06295483	1
Fagron	Rutosídeo tri-hidratado	L14050127	1

S

Supplier	Substance	Batch	Spectra
Bombastus	Sabugueiro	275393	4
Bahnhof-Apotheke	Sabugueiro	17-121112	1
Bombastus	Sabugueiro	265631	1
Bombastus	Sabugueiro	289348	1
Bombastus	Sabugueiro	279216	3
Caelo	Sabugueiro	12221902	11
Caelo	Sabugueiro	10291308	2
Caelo	Sabugueiro	10291312	2
Caelo	Sabugueiro	12221904	10
Caelo	Sabugueiro	1571a121022	1
Caelo	Sabugueiro	31051301	1
Caelo	Sabugueiro	12221905	7
Caelo	Sabugueiro	12221906	1
Caelo	Sabugueiro	12221907	4
Caelo	Sabugueiro	14111317	1
Caelo	Sabugueiro	5122013d	1
Caelo	Sabugueiro	12221909	1
Caelo	Sabugueiro	13244601	4
Caelo	Sabugueiro	13244602	2
Caelo	Sabugueiro	12221910	2
Caelo	Sabugueiro	1571A121022	14
Caelo	Sabugueiro	10291309	3
Caelo	Sabugueiro	12221904-3360319071	1
Caesar/Noweda	Sabugueiro	4910A-01471	1
Finze	Sabugueiro	9297415	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Galke	Sabugueiro	21934	1
Gehe	Sabugueiro	1250213	1
Gehe	Sabugueiro	1090413	1
Klenk	Sabugueiro	1571A141126	1
Klenk	Sabugueiro	1571A110223	16
Klenk	Sabugueiro	16061201	1
Klenk	Sabugueiro	26061201	1
Klenk	Sabugueiro	21091201	1
Klenk	Sabugueiro	1571A110125	2
Klenk	Sabugueiro	13021301	1
Klenk	Sabugueiro	1571A121121	20
Klenk	Sabugueiro	1571A1202015	1
Klenk	Sabugueiro	A121121	1
Klenk	Sabugueiro	A120215	1
Klenk	Sabugueiro	1571A130627	2
Klenk	Sabugueiro	1571A-110223	1
Klenk	Sabugueiro	1571a120215	1
Klenk	Sabugueiro	1571A130930	3
Klenk	Sabugueiro	1571a1211	1
Klenk	Sabugueiro	1571A120215	4
Caelo	Sabugueiro	1029310	1
Bombastus	Sabugueiro	269873	2
Caelo	Sabugueiro	10291310	5
Wolf	Sabugueiro	E-738	1
Wolf	Sabugueiro	22749	1
Wolf	Sabugueiro	22765	1
Wolf	Sabugueiro	B-810	1
Caelo	Salsa, esfregada	12376601	2
Caelo	Salsa, esfregada	51978126	1
Caelo	Salsa, esfregada	12376603	2
Caelo	Salsa, esfregada	12376602	2
Caelo	Salsaparrilha, cortada	13079201	1
Klenk	Salsaparrilha, cortada	6561B111108	1
Klenk	Salsaparrilha, cortada	B111108	1
Galke	Sanícula, cortada	23097	1
bohn	Segurelha, esfregada	12177208	1
Caelo	Segurelha, esfregada	12177203	7
Caelo	Segurelha, esfregada	12200801	1
Caelo	Segurelha, esfregada	12177201	1
Caelo	Segurelha, esfregada	12177207	2
Caelo	Segurelha, esfregada	13172404	2
Hepart AG	Segurelha, esfregada	12177205	3
Allianz Healthcare	Semente de abóbora	16081210	1
Caelo	Semente de abóbora	12249001	2
Caelo	Semente de abóbora	14186905	1
Caelo	Semente de abóbora	14186910	1
Caelo	Semente de abóbora	16081202	1
Caelo	Semente de abóbora	16081206	2
Caelo	Semente de abóbora	140736306	1
Caelo	Semente de abóbora	122490911	1
Caelo	Semente de abóbora	12249011	2
Caelo	Semente de abóbora	14073603	1
sanacorp	Semente de abóbora	14186909	1
Sanacorp	Semente de abóbora	16081212	1
Akazie	Semente de cominho preto	20.09.2015	1
Caelo	Semente de cominho preto	10121916	1
Caelo	Semente de cominho preto	10121915	1
Caelo	Semente de cominho preto	11233502	2
Caelo	Semente de cominho preto	12358901	2
Caelo	Semente de cominho preto	12358906	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Semente de cominho preto	13326405	2
Caelo	Semente de cominho preto	13326406	1
Caelo	Semente de cominho preto	14359903	3
Caelo	Semente de cominho preto	14359905	1
Caelo	Semente de cominho preto	16115710	1
Caelo	Semente de cominho preto	12358903	2
Caelo	Semente de cominho preto	16115708	3
Caelo	Semente de cominho preto	15300401	3
Caelo	Semente de cominho preto	16115706	1
Caelo	Semente de cominho preto	11233507	1
Caelo	Semente de cominho preto	13122013b	1
Caelo	Semente de cominho preto	16115703	2
Chiesi/Phönix	Semente de cominho preto	14359906	2
Hepart AG	Semente de cominho preto	20720,kbA	1
Caelo	Semente de cominho preto	12358902	1
Caelo	Semente de cominho preto	12358904	1
Klenk	Semente de cominho preto	7330A120703	1
Klenk	Semente de cominho preto	A120703	1
Caelo	Semente de cominho preto	11233503	1
Spinnrad	Semente de cominho preto	11931059	1
Spinnrad/Phoenix	Semente de cominho preto	613310592	1
Wolf	Semente de cominho preto		1
Wolf	Semente de cominho preto	20720	8
Wolf	Semente de cominho preto	B-471	1
Wolf	Semente de cominho preto	207204	1
Wolf	Semente de cominho preto	L310F141b	6
Wolf	Semente de cominho preto	L402F1713	1
Wolf	Semente de cominho preto	L402F171b	3
Caelo	Semente de mostarda preta, ...	17196303	4
Klenk	Semente de mostarda preta, ...	7434A120712	1
Caelo	Semente de mostarda preta, ...	16051810	4
Caelo	Semente de mostarda preta, ...	12009702	4
Caelo	Semente de mostarda preta, ...	12009706	1
Caelo	Semente de mostarda preta, ...	12208602	5
Caelo	Semente de mostarda preta, ...	12208601	3
Caelo	Semente de mostarda preta, ...	12350202	16
Caelo	Semente de mostarda preta, ...	12350205	2
Caelo	Semente de mostarda preta, ...	12350208	7
Caelo	Semente de mostarda preta, ...	12350204	2
Caelo	Semente de mostarda preta, ...	12350210	1
Caelo	Semente de mostarda preta, ...	12350211	3
Caelo	Semente de mostarda preta, ...	13097705	6
Caelo	Semente de mostarda preta, ...	12350209	1
Caelo	Semente de mostarda preta, ...	13097704	4
Caelo	Semente de mostarda preta, ...	13358302	13
Caelo	Semente de mostarda preta, ...	25011401	1
Caelo	Semente de mostarda preta, ...	13358304	4
Caelo	Semente de mostarda preta, ...	23061401	1
Caelo	Semente de mostarda preta, ...	14162810	2
Caelo	Semente de mostarda preta, ...	14293702	6
Caelo	Semente de mostarda preta, ...	14162802	1
Caelo	Semente de mostarda preta, ...	15131102	3
Caelo	Semente de mostarda preta, ...	15214703	1
Caelo	Semente de mostarda preta, ...	15214707	1
Caelo	Semente de mostarda preta, ...	15214713	2
Caelo	Semente de mostarda preta, ...	16051807	1
Caelo	Semente de mostarda preta, ...	12208604	3
Caelo	Semente de mostarda preta, ...	11276701	1
Caelo	Semente de mostarda preta, ...	12009703	1
Caelo	Semente de mostarda preta, ...	15214714	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Semente de mostarda preta, ...	16051807	1
Caelo	Semente de mostarda preta, ...	15131101	1
Caelo	Semente de mostarda preta, ...	16272704	2
Caelo	Semente de mostarda preta, ...	14293706	1
Caelo	Semente de mostarda preta, ...	15214707	2
Caelo	Semente de mostarda preta, ...	13097701	11
Caelo	Semente de mostarda preta, ...	13097702	4
Caelo	Semente de mostarda preta, ...	2015Q-02244	1
Caelo	Semente de mostarda preta, ...	17196306	1
Caelo	Semente de mostarda preta, ...	14162807	3
Caelo	Semente de mostarda preta, ...	14162810	3
Caelo	Semente de mostarda preta, ...	14245601	1
Caelo	Semente de mostarda preta, ...	14293701	2
Caelo	Semente de mostarda preta, ...	14293710	2
Caelo	Semente de mostarda preta, ...	15131104	1
Caelo	Semente de mostarda preta, ...	15214703	7
Caelo	Semente de mostarda preta, ...	16272703	6
Caelo	Semente de mostarda preta, ...	16272707	4
Caelo	Semente de mostarda preta, ...	16333501	2
Caelo	Semente de mostarda preta, ...	1633503	1
Caelo	Semente de mostarda preta, ...	17196301	1
Caelo	Semente de mostarda preta, ...	15131105	1
Caelo	Semente de mostarda preta, ...	15214706	3
Caelo	Semente de mostarda preta, ...	14162808	1
Caelo	Semente de mostarda preta, ...	14293713	1
Caelo	Semente de mostarda preta, ...	15214708	4
Caelo	Semente de mostarda preta, ...	12350202-3369319012	1
Caelo	Semente de mostarda preta, ...	13097706	2
Caelo	Semente de mostarda preta, ...	12350207	5
Caesar / Ebert & Jacobi	Semente de mostarda preta, ...	16051809	1
Caesar/ Noweda	Semente de mostarda preta, ...	14293711	3
Caelo	Semente de mostarda preta, ...	16333503	3
Caelo	Semente de mostarda preta, ...	17276404	1
Klenk	Semente de mostarda preta, ...	A130422	1
Klenk	Semente de mostarda preta, ...	7434A130422	3
Klenk	Semente de mostarda preta, ...	7434A140923	2
Klenk	Semente de mostarda preta, ...	7434A150608	4
Klenk	Semente de mostarda preta, ...	7434a150608	1
Noweda/Henry Lamotte	Semente de mostarda preta, ...	1493708	1
Caelo	Semente de mostarda preta, ...	16051802	3
Caelo	Semente de mostarda, branca...	7254a110823	1
Caelo	Semente de mostarda, branca...	12375701	1
Caelo	Semente de mostarda, branca...	12375705	1
Caelo	Semente de mostarda, branca...	12375706	2
Caelo	Semente de mostarda, branca...	12375704	1
Caelo	Semente de mostarda, branca...	12375705	4
Caelo	Semente de mostarda, branca...	13224804	3
Caelo	Semente de mostarda, branca...	13224801	1
Caelo	Semente de mostarda, branca...	12375702	1
Klenk	Semente de mostarda, branca...	7254A141202	1
Caelo	Semente de mostarda, branca...	11114409	1
Caelo	Semente de mostarda, preta	12189307	1
Caelo	Semente de mostarda, preta	14057702	1
Caelo	Semente de mostarda, preta	16139102	1
Caelo	Semente de mostarda, preta	13038904	1
Klenk	Semente de mostarda, preta	7430A120813	2
Audor Pharma	Semente de psílio	15190313	2
Bahnhof-Apotheke	Semente de psílio	3-121005	1
Caelo	Semente de psílio	10291205	1
Caelo	Semente de psílio	12140301	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Semente de psílio	10291206	1
Caelo	Semente de psílio	12185504	10
Caelo	Semente de psílio	10291204	1
Caelo	Semente de psílio	12185509	5
Caelo	Semente de psílio	12185508	4
Caelo	Semente de psílio	12276510	1
Caelo	Semente de psílio	13305904	2
Caelo	Semente de psílio	13305903	1
Caelo	Semente de psílio	13305906	2
Caelo	Semente de psílio	13305910	4
Caelo	Semente de psílio	10061503	1
Caelo	Semente de psílio	15190304	3
Caelo	Semente de psílio	10291207	6
Caelo	Semente de psílio	13234310	3
Caelo	Semente de psílio	12185503	3
Caelo	Semente de psílio	13234309	1
Caelo	Semente de psílio	7380a120911	1
Caelo	Semente de psílio	11185811	4
Caelo	Semente de psílio	15190303	4
Caelo	Semente de psílio	11185803	1
Caelo	Semente de psílio	13305907	5
Caelo	Semente de psílio	15190306	2
Caelo	Semente de psílio	15321007	1
Caelo	Semente de psílio	12185502	1
Caesar/Noweda	Semente de psílio	11185817	3
Caesar/Noweda	Semente de psílio	12276501	3
Galke	Semente de psílio	20968	2
Galke	Semente de psílio	22989	7
Klenk	Semente de psílio	7380A150520	7
Klenk	Semente de psílio	7560a120330	1
Klenk	Semente de psílio	A120911	1
Klenk	Semente de psílio	A120109	1
Klenk	Semente de psílio	A130128	1
Klenk	Semente de psílio	7560A130418	1
Klenk	Semente de psílio	7380A150929	4
Klenk	Semente de psílio	7380A161018	2
Klenk	Semente de psílio	7380A110317	1
Klenk	Semente de psílio	7380A111018	1
Klenk	Semente de psílio	7380A130128	6
Klenk	Semente de psílio	7380A120109	24
Klenk	Semente de psílio	7380a111018	1
Klenk	Semente de psílio	7380a120109	3
Klenk	Semente de psílio	7380A120911	16
Klenk	Semente de psílio	7560A140203	1
Caelo	Semente de salsa	PrüfNr.2814A-01550	1
Klenk	Semente de salsa	7370A091120	2
Klenk	Semente de salsa	7370A09120	1
Caelo	Semente de urtiga	12131505	1
Caelo	Semente de urtiga	13010607	1
Caelo	Semente de urtiga	20111301	1
Caelo	Semente de urtiga	13010612	2
Caelo	Semente de urtiga	15261608	1
Caelo	Semente de urtiga	17282601	1
Caelo	Semente de urtiga	15290602	1
Caelo	Semente de urtiga	16327001	3
Caelo	Semente de urtiga	16327003	1
Euro OTC	Semente de urtiga	12131507	2
Euro OTC	Semente de urtiga	7470A141021	2
Klenk	Semente de urtiga	7470A110418	1
Klenk	Semente de urtiga	2021505	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Semente de urtiga	7470A151009	2
Klenk	Semente de urtiga	7470A170130	1
Klenk	Semente de urtiga	7470A160928	2
Sanacorp	Semente de urtiga	13010602	1
Caelo	Sempre-viva	1024407	1
Caelo	Sempre-viva	10244407	1
Caelo	Sempre-viva	12170605	2
Caelo	Sempre-viva	15029505	1
Caelo	Sempre-viva	11293101	4
Caelo	Sempre-viva	512U-01473	1
Caelo	Sempre-viva	12170603	1
Klenk	Sempre-viva	1591A110511	13
Klenk	Sempre-viva	1591A-110511	1
Caelo	Sempre-viva	12170602	2
VDL	Sempre-viva	10244406	1
Caelo	Sequoia africana, cortada	12049608	2
Caelo	Sequoia africana, cortada	12041403	1
Caelo	Sequoia africana, cortada	13106901	1
Caelo	Sequoia africana, cortada	12049607	2
Klenk	Sequoia africana, cortada	5961B111219	1
Caelo	Sinapis alba, semente	15120304	1
Caelo	Sódio 4-hidroxibenzoato de …	17051903	2
Caelo	Sódio 4-hidroxibenzoato de …	18060803	1
Caelo	Sódio 4-hidroxibenzoato de …	18060801	1
Caelo	Sódio 4-hidroxibenzoato de …	19143902	2
Caelo	Softisan® 601	15184901	1
Caelo	Softisan® 601	13296104	1
Caelo	Softisan® 601	14099608	1
Caesar & Loretz GmbH	Softisan® 601	18197002	2
-	Stellaria media, cortada	2011A-01686	1
Caelo	Stellaria media, cortada	13040501	1
Caelo	Stellaria media, cortada	13040503	1
Caelo	Stellaria media, cortada	13254403	2
Caelo	Stellaria media, cortada	13254401	1
Caelo	Stellaria media, cortada	4551B130902	1
Caelo	Stellaria media, cortada	14212411	1
Caelo	Stellaria media, cortada	16143603	1
Caelo	Stellaria media, cortada	13040502-3283310662	1
Caelo	Stellaria media, cortada	16143608	2
Caelo	Stellaria media, cortada	13040502	2
Caelo	Stellaria media, cortada	13254404	1
Caelo	Stellaria media, cortada	13040504	1
Klenk	Stellaria media, cortada	4551b110222	1
Klenk	Stellaria media, cortada	4551B090528	1
Phoenix	Stellaria media, cortada	18100704	1
Caelo	Stellaria media, cortada	14212405	1
Caelo	Sulfamerazina	10218401	1
Fagron	Sulfanilamida	11L01-No8	1
Dermapharm	Sulfato de 8-quinolinol mon…	140804	1
Dermapharm	Sulfato de 8-quinolinol mon…	100804	1
Fagron	Sulfato de 8-quinolinol mon…	10F01-N15	1
Fagron	Sulfato de 8-quinolinol mon…	11L08-N07	2
Fagron	Sulfato de 8-quinolinol mon…	11/09-N09	1
Fagron	Sulfato de 8-quinolinol mon…	11L19-N14	1
Fagron	Sulfato de 8-quinolinol mon…	13/21-N23	1
Fagron	Sulfato de 8-quinolinol mon…	13D24-N11	1
Fagron	Sulfato de 8-quinolinol mon…	13G10-N06	1
Fagron	Sulfato de 8-quinolinol mon…	12A04-N05	1
Fagron	Sulfato de 8-quinolinol mon…	11I09-N09	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sulfato de 8-quinolinol mon…	13A04-N05	1
Fagron	Sulfato de 8-quinolinol mon…	12D26-N04	1
Fagron	Sulfato de 8-quinolinol mon…	12H21-N08	1
Fagron	Sulfato de 8-quinolinol mon…	13032014C	1
Dermapharm	Sulfato de 8-quinolinol mon…	120905	1
siehe WE-Prüfprotokoll	Sulfato de 8-quinolinol mon…	96/09	1
Caelo	Sulfato de alumínio e potássio	14263804	1
Alliance Health	Sulfato de alumínio e potássio	13025401	3
Alliance Healthcare	Sulfato de alumínio e potássio	13025404	1
Anzag	Sulfato de alumínio e potássio	1218441	1
Caelo	Sulfato de alumínio e potássio	1218411	1
Caelo	Sulfato de alumínio e potássio	12022444	1
Caelo	Sulfato de alumínio e potássio	12022404	1
Caelo	Sulfato de alumínio e potássio	510211092	1
Caelo	Sulfato de alumínio e potássio	11017211	1
Caelo	Sulfato de alumínio e potássio	12022406	2
Caelo	Sulfato de alumínio e potássio	12184401	2
Caelo	Sulfato de alumínio e potássio	12184407	3
Caelo	Sulfato de alumínio e potássio	504311092	1
Caelo	Sulfato de alumínio e potássio	90033229	1
Caelo	Sulfato de alumínio e potássio	12144605	4
Caelo	Sulfato de alumínio e potássio	12184408	3
Caelo	Sulfato de alumínio e potássio	12144607	2
Caelo	Sulfato de alumínio e potássio	12239102	2
Caelo	Sulfato de alumínio e potássio	13025401	3
Caelo	Sulfato de alumínio e potássio	12184411	1
Caelo	Sulfato de alumínio e potássio	2713Q1092	1
Caelo	Sulfato de alumínio e potássio	13025404	3
Caelo	Sulfato de alumínio e potássio	15172501	1
Caelo	Sulfato de alumínio e potássio	12184401	1
Caelo	Sulfato de alumínio e potássio	12144602	1
Caelo	Sulfato de alumínio e potássio	12184406	2
Caelo	Sulfato de alumínio e potássio	11254805	1
Caelo	Sulfato de alumínio e potássio	11218611	2
Caelo	Sulfato de alumínio e potássio	12184402	3
Caelo	Sulfato de alumínio e potássio	13098702	1
Caelo	Sulfato de alumínio e potássio	12184407	5
Caelo	Sulfato de alumínio e potássio	12022409	1
Caelo	Sulfato de alumínio e potássio	12022401	1
Caelo	Sulfato de alumínio e potássio	12022406	1
Caesar/Noweda	Sulfato de alumínio e potássio	12184411	2
Euro OTC	Sulfato de alumínio e potássio	1004046-02	1
Fagron	Sulfato de alumínio e potássio	A1-063-Al	1
Fagron	Sulfato de alumínio e potássio	12/24-M02	1
Fagron	Sulfato de alumínio e potássio	103638	1
Fagron	Sulfato de alumínio e potássio	A1-063-AL	1
Fagron	Sulfato de alumínio e potássio	13D08-N01	1
Caelo	Sulfato de alumínio e potássio	12|24-M03	1
Fagron	Sulfato de alumínio e potássio	13D29-N04	1
Sanacorp	Sulfato de alumínio e potássio	12184402	2
Caelo	Sulfato de alumínio e potássio	12144603	1
Fagron	Sulfato de alumínio e potássio	12I24-M03	1
Caelo	Sulfato de cálcio di-hidratado	10132403	1
Caelo	Sulfato de cálcio di-hidratado	12316301	1
Caelo	Sulfato de cálcio hemi-hidratado	14101701	1
Caelo	Sulfato de cálcio hemi-hidratado	9246320	1
Caelo	Sulfato de cobre (II) penta…	3411M-01317	1
Caelo	Sulfato de cobre (II) penta…	12157107	1
Caelo	Sulfato de cobre (II) penta…	10L15-N06	1
Caelo	Sulfato de cobre (II) penta…	3211M-01317	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfato de cobre (II) penta…	2913U-01317	1
Fagron	Sulfato de cobre (II) penta…	13A25-N06	1
Caelo	Sulfato de ferro (III) hidratado	12175908	1
Caelo	Sulfato de ferro (III) hidratado	1512210007	1
Caelo	Sulfato de ferro (III) hidratado	10354412	1
Caelo	Sulfato de ferro (III) hidratado	12175906	1
Caelo	Sulfato de ferro (III) hidratado	10354404	1
Caelo	Sulfato de ferro (III) hidratado	10354415	1
Caelo	Sulfato de magnésio seco	11265902	1
Caelo	Sulfato de magnésio seco	11265903	1
Caelo	Sulfato de magnésio seco	12157202	1
Caelo	Sulfato de magnésio seco	M-220413-2	1
Caelo	Sulfato de magnésio seco	12157207	1
Caelo	Sulfato de magnésio seco	12157208	1
Caelo	Sulfato de magnésio seco	10213213	2
Caelo	Sulfato de magnésio seco	11265908	2
Caelo	Sulfato de morfina	17331507	1
Caelo	Sulfato de morfina	17331510	4
Caelo	Sulfato de quinolinol sulfa…	7051305	1
Caelo	Sulfato de quinolinol sulfa…	13071104	4
Caelo	Sulfato de quinolinol sulfa…	13403501	4
Caelo	Sulfato de quinolinol sulfa…	15147701	3
Caelo	Sulfato de quinolinol sulfa…	15147714	1
Caelo	Sulfato de quinolinol sulfa…	13403506	15
Caelo	Sulfato de quinolinol sulfa…	13071101	2
Caelo	Sulfato de quinolinol sulfa…	15147706	5
Caelo	Sulfato de quinolinol sulfa…	10281601	1
Caelo	Sulfato de quinolinol sulfa…	13071106	1
Caelo	Sulfato de quinolinol sulfa…	15147708	4
Caelo	Sulfato de quinolinol sulfa…	16221809	6
Caelo	Sulfato de quinolinol sulfa…	13403501	3
Caelo	Sulfato de quinolinol sulfa…	9106304	1
Caelo	Sulfato de quinolinol sulfa…	13403513	1
Caelo	Sulfato de quinolinol sulfa…	15147704	4
Caelo	Sulfato de quinolinol sulfa…	16221807	6
Caelo	Sulfato de quinolinol sulfa…	16221811	2
Dermapharm	Sulfato de quinolinol sulfa…	100804	12
Dermapharm	Sulfato de quinolinol sulfa…	140804	82
Dermapharm	Sulfato de quinolinol sulfa…	120905	43
Dermapharm	Sulfato de quinolinol sulfa…	1470804	1
Ebert-Jacobi	Sulfato de quinolinol sulfa…	16221804	2
Lieber Leyh	Sulfato de quinolinol sulfa…	1605110096	1
Nachprüfung	Sulfato de quinolinol sulfa…	2812U03423	1
Nachprüfung	Sulfato de quinolinol sulfa…	13071104	1
Noweda	Sulfato de quinolinol sulfa…	140804	2
Phönix Gotha	Sulfato de quinolinol sulfa…	120905	10
	SyrSpend® SF Alka	22J04-F06-383652	20
	SyrSpend® SF Alka	22J04-F06-3636502	3
	SyrSpend® SF Alka	F0238363009	1
	SyrSpend® SF Alka	F07-3819306	1
	SyrSpend® SF Alka	22K17-F04-384631	1
	SyrSpend® SF Alka	22j31-F01-526993	1
	SyrSpend® SF Alka	22J04-F11-383746	7
	SyrSpend® SF Alka	22J04-F06-383652	1
	SyrSpend® SF Alka	22J04F02383639	1
	SyrSpend® SF Alka	22J04-F08-383658	4
	SyrSpend® SF Alka	23A18-F07-384725	6
	SyrSpend® SF Alka	F01-3847703	1
	SyrSpend® SF Alka	23B16-F01-384773	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	SyrSpend® SF Alka	23B16-F03-384777	2
	SyrSpend® SF Alka	23B16-F02-384774	2
	SyrSpend® SF Alka	22K18-F01-384185	1
AHD	SyrSpend® SF Alka	22K17-F05-384376	2
Fagron	SyrSpend® SF Alka	15K03-B01-525173	1
Fagron	SyrSpend® SF Alka	19F06-b02-363789	2
Fagron	SyrSpend® SF Alka	18a26b05346410	1
Fagron	SyrSpend® SF Alka	19d29b07362182	1
Caelo	SyrSpend® SF Alka	18871B06	1
Caelo	SyrSpend® SF Alka	353473	1
Caelo	SyrSpend® SF Alka	720026-000	1
Caelo	SyrSpend® SF Alka	12B23-B07-305668	1
Caelo	SyrSpend® SF Alka	18125-B15-357803	2
Fagron	SyrSpend® SF Alka	14J22-B40-311723	2
Fagron	SyrSpend® SF Alka	17D11-B04-332593	8
Fagron	SyrSpend® SF Alka	17D11-B04	2
Fagron	SyrSpend® SF Alka	17D11-bo4-332593	1
Fagron	SyrSpend® SF Alka	17F14-B02-335945	5
Fagron	SyrSpend® SF Alka	18A26-B05-346410	5
Fagron	SyrSpend® SF Alka	18821-b08-347192	1
Fagron	SyrSpend® SF Alka	18C-B11-350851	1
Fagron	SyrSpend® SF Alka	18H01-B12-353473	35
Fagron	SyrSpend® SF Alka	18/25-B15-357803	1
Fagron	SyrSpend® SF Alka	18L21-B11-359901	23
Fagron	SyrSpend® SF Alka	18L25-B15-357803	1
Fagron	SyrSpend® SF Alka	18821-808-147192	1
Fagron	SyrSpend® SF Alka	18L21B11359901	1
Fagron	SyrSpend® SF Alka	19F12-B07-526149	8
Fagron	SyrSpend® SF Alka	19F12-B07	2
Fagron	SyrSpend® SF Alka	B02-3637809	4
Fagron	SyrSpend® SF Alka	19F12	1
Fagron	SyrSpend® SF Alka	19Ko7-F04-367548	1
Fagron	SyrSpend® SF Alka	20B818-F03-369574	2
Fagron	SyrSpend® SF Alka	20B25-F06-369913	31
Fagron	SyrSpend® SF Alka	20825-F07-3669914	2
Fagron	SyrSpend® SF Alka	20817-F03	1
Fagron	SyrSpend® SF Alka	20B25-F07-369914	9
Fagron	SyrSpend® SF Alka	B04-3640507	1
Fagron	SyrSpend® SF Alka	F11-3742709	3
Fagron	SyrSpend® SF Alka	F1137427009	3
Fagron	SyrSpend® SF Alka	20825-F07	1
Fagron	SyrSpend® SF Alka	20D15-F08-371028	2
Fagron	SyrSpend® SF Alka	18J25-B15357803	1
Fagron	SyrSpend® SF Alka	F12-3748002	1
Fagron	SyrSpend® SF Alka	7-378133	1
Fagron	SyrSpend® SF Alka	21B26-F07378133	1
Fagron	SyrSpend® SF Alka	20D15-F08	1
Fagron	SyrSpend® SF Alka	21F24F01379228	1
Fagron	SyrSpend® SF Alka	21F24-F03-379228	1
Fagron	SyrSpend® SF Alka	21F08-F03-378828	1
Fagron	SyrSpend® SF Alka	21F24-F04	2
Fagron	SyrSpend® SF Alka	20D16-F06	1
Fagron	SyrSpend® SF Alka	21I01-F02	1
Fagron	SyrSpend® SF Alka	21H16-F06-379894	27
Fagron	SyrSpend® SF Alka	21H16-F06	1
Fagron	SyrSpend® SF Alka	21B26-F06	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	22A12-F20-381408	6
Fagron	SyrSpend® SF Alka	22B04-F06	2
Fagron	SyrSpend® SF Alka	22B04-F06-381564	13
Fagron	SyrSpend® SF Alka	22B04F06-381564	1
Fagron	SyrSpend® SF Alka	21H16F06379894	1
Fagron	SyrSpend® SF Alka	22804-F06-381564	1
Fagron	SyrSpend® SF Alka	802-3637809	1
Fagron	SyrSpend® SF Alka	19F12-B04-36-4057	1
Fagron	SyrSpend® SF Alka	F03-3695704	2
Fagron	SyrSpend® SF Alka	21926-F07-378133	1
Fagron	SyrSpend® SF Alka	22B04F05-3819009	1
Fagron	SyrSpend® SF Alka	21L-07-F05-381032	1
Fagron	SyrSpend® SF Alka	18j25-B15	1
Fagron	SyrSpend® SF Alka	21L07-F05	8
Fagron	SyrSpend® SF Alka	21H16-F06	1
Fagron	SyrSpend® SF Alka	720026-0000	2
Fagron	SyrSpend® SF Alka	21A21-F01	5
Fagron	SyrSpend® SF Alka	318828	1
Fagron	SyrSpend® SF Alka	21101-F02-380031	1
Fagron	SyrSpend® SF Alka	F02-3800301	1
Fagron	SyrSpend® SF Alka	18H01-B12353473	1
Fagron	SyrSpend® SF Alka	17F14B02-335945	1
Fagron	SyrSpend® SF Alka	18H01-b12	1
Fagron	SyrSpend® SF Alka	19F12-804-364057	1
Fagron	SyrSpend® SF Alka	21L07-F04-381033	2
Fagron	SyrSpend® SF Alka	20F18-F14-379344	1
Fagron	SyrSpend® SF Alka	22B04-F05-381909	2
Fagron	SyrSpend® SF Alka	22A12-F21	1
Fagron	SyrSpend® SF Alka	22A12-F24-382104	5
Fagron	SyrSpend® SF Alka	22A12-F22-382195	16
Fagron	SyrSpend® SF Alka	22J04-F0-2383639	1
Fagron	SyrSpend® SF Alka	22B04-F05-381975	1
Fagron	SyrSpend® SF Alka	21101-F02	1
Fagron	SyrSpend® SF Alka	18H01-812353473	1
Fagron	SyrSpend® SF Alka	19D29-Bo7-362182	1
Fagron	SyrSpend® SF Alka	19D29B07	1
Fagron	SyrSpend® SF Alka	19D29807362182	1
Fagron	SyrSpend® SF Alka	19F06-B002	1
Fagron	SyrSpend® SF Alka	19k07fo4	1
Fagron	SyrSpend® SF Alka	20825f0625F06	1
Fagron	SyrSpend® SF Alka	20G03-F12-374282	7
Fagron	SyrSpend® SF Alka	17F14802-335945	1
Fagron	SyrSpend® SF Alka	19D29-B07	1
Fagron	SyrSpend® SF Alka	19F12-B04	6
Fagron	SyrSpend® SF Alka	17D11-804-332593	1
Fagron	SyrSpend® SF Alka	181C13-B11-350851	1
Fagron	SyrSpend® SF Alka	19F06-B02-363789	29
Fagron	SyrSpend® SF Alka	19D29-807	1
Fagron	SyrSpend® SF Alka	21B26-F07-378133	9
Fagron	SyrSpend® SF Alka	F03-3788208	1
Fagron	SyrSpend® SF Alka	22B04-F07-381936	4
Fagron	SyrSpend® SF Alka	22B04-F06-381564	1
Fagron	SyrSpend® SF Alka	19F06-B02	7
Fagron	SyrSpend® SF Alka	19K07-F04	4
Fagron	SyrSpend® SF Alka	2085-F06	1
Fagron	SyrSpend® SF Alka	21826-F08	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	21101_F-02	1
Fagron	SyrSpend® SF Alka	20818-F03-369574	3
Fagron	SyrSpend® SF Alka	21B26-F06	2
Fagron	SyrSpend® SF Alka	17F14-B05	1
Fagron	SyrSpend® SF Alka	21F08-F04-378832	5
Fagron	SyrSpend® SF Alka	22A12F20381408	1
Fagron	SyrSpend® SF Alka	22A12F21526828	1
Fagron	SyrSpend® SF Alka	22A12-F21-526828	3
Fagron	SyrSpend® SF Alka	22J31-F01-526993	3
Fagron	SyrSpend® SF Alka	21F24-F03-526598	3
Fagron	SyrSpend® SF Alka	19D29-B11-363786	8
Fagron	SyrSpend® SF Alka	18A26-Bo5-346410	1
Fagron	SyrSpend® SF Alka	19029-B07-362182	1
Fagron	SyrSpend® SF Alka	21H16-F06-0000	1
Fagron	SyrSpend® SF Alka	17F14-B05-525556	2
Fagron	SyrSpend® SF Alka	19K07-F04-367548	5
Fagron	SyrSpend® SF Alka	20B25-F06_369913	1
Fagron	SyrSpend® SF Alka	20825-F06-369913	3
Fagron	SyrSpend® SF Alka	20818F03	1
Fagron	SyrSpend® SF Alka	21A21-F01-376829	18
Fagron	SyrSpend® SF Alka	21B26-F08	2
Fagron	SyrSpend® SF Alka	379672	1
Fagron	SyrSpend® SF Alka	21101-F02-380031	4
Fagron	SyrSpend® SF Alka	21L07-F05-381032	41
Fagron	SyrSpend® SF Alka	21L07F05381032	1
Fagron	SyrSpend® SF Alka	22804-F06	1
Fagron	SyrSpend® SF Alka	F07-3788300	2
Fagron	SyrSpend® SF Alka	21826-F08-379141	2
Fagron	SyrSpend® SF Alka	18C13_B11_350851	1
Fagron	SyrSpend® SF Alka	F07-3699104	3
Fagron	SyrSpend® SF Alka	20B18F03369574	1
Fagron	SyrSpend® SF Alka	20825-F07-369914	2
Fagron	SyrSpend® SF Alka	17D29-B11	1
Fagron	SyrSpend® SF Alka	6369913	1
Fagron	SyrSpend® SF Alka	20G03-F12	2
Fagron	SyrSpend® SF Alka	14I22-B40-311723	1
Fagron	SyrSpend® SF Alka	18B21-B08-347192	3
Fagron	SyrSpend® SF Alka	20B18-F03	3
Fagron	SyrSpend® SF Alka	19K007-F04	1
Fagron	SyrSpend® SF Alka	21F24-F01-37928	1
Fagron	SyrSpend® SF Alka	21F24-F03526598	1
Fagron	SyrSpend® SF Alka	20G03-F09-526400	2
Fagron	SyrSpend® SF Alka	20D16-F01	1
Fagron	SyrSpend® SF Alka	20B18-F03-	1
Fagron	SyrSpend® SF Alka	21A21-376829	3
Fagron	SyrSpend® SF Alka	20B25-F07	9
Fagron	SyrSpend® SF Alka	20G03-F11	3
Fagron	SyrSpend® SF Alka	18J21B113659901	1
Fagron	SyrSpend® SF Alka	18L21-B113659901	1
Fagron	SyrSpend® SF Alka	19F12-B04-364057	16
Fagron	SyrSpend® SF Alka	20B18-F03-369574	10
Fagron	SyrSpend® SF Alka	20G03-F11-374279	21
Fagron	SyrSpend® SF Alka	F01-376829	2
Fagron	SyrSpend® SF Alka	21F08-F03	3
Fagron	SyrSpend® SF Alka	21I01-F02-380031	28
Fagron	SyrSpend® SF Alka	FO6-3798904	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	22J04-F02-383639	10
Fagron	SyrSpend® SF Alka	18A26-B05	1
Fagron	SyrSpend® SF Alka	18B21-B08	3
Fagron	SyrSpend® SF Alka	18821-B08-347192	5
Fagron	SyrSpend® SF Alka	18C13-B11	6
Fagron	SyrSpend® SF Alka	18H01-B12	7
Fagron	SyrSpend® SF Alka	18J25-B15-357803	23
Fagron	SyrSpend® SF Alka	18J25-B15	6
Fagron	SyrSpend® SF Alka	18L21-B11	12
Fagron	SyrSpend® SF Alka	19F12-BO4-364057	4
Fagron	SyrSpend® SF Alka	19K07-F04-367548	6
Fagron	SyrSpend® SF Alka	19-F12-B04	1
Fagron	SyrSpend® SF Alka	F06-3699103	3
Fagron	SyrSpend® SF Alka	20B25-F06	4
Fagron	SyrSpend® SF Alka	F06-369913	1
Fagron	SyrSpend® SF Alka	20825-F07369914	2
Fagron	SyrSpend® SF Alka	F01-3768209	2
Fagron	SyrSpend® SF Alka	21F08-F03-378828	21
Fagron	SyrSpend® SF Alka	21B26-F08-379141	10
Fagron	SyrSpend® SF Alka	F08-3791401	2
Fagron	SyrSpend® SF Alka	21F08-F04	1
Fagron	SyrSpend® SF Alka	21F24-F04-379672	4
Fagron	SyrSpend® SF Alka	F0538103002	1
Fagron	SyrSpend® SF Alka	F04-3815505	1
Fagron	SyrSpend® SF Alka	18H13-B12-353473	1
Fagron	SyrSpend® SF Alka	16B03-B07-525234	1
Fagron	SyrSpend® SF Alka	18C13-B11-350851	9
Fagron	SyrSpend® SF Alka	21A21-FO1	1
Fagron	SyrSpend® SF Alka	F07-3781303	1
Fagron	SyrSpend® SF Alka	21F08F03378828	1
Fagron	SyrSpend® SF Alka	21A21-F01-.376829	1
Fagron	SyrSpend® SF Alka	21F24-F01-379228	17
Fagron	SyrSpend® SF Alka	B07-5261409	3
Fagron	SyrSpend® SF Alka	20825-O6-3669913	1
Fagron	SyrSpend® SF Alka	20Go3-f12-374282	1
Fagron	SyrSpend® SF Alka	20B25-FO7-369914	1
Fagron	SyrSpend® SF Alka	21F24-FO1	1
Fagron	SyrSpend® SF Alka	2IL07-F05-381032	1
Fagron	SyrSpend® SF Alka	22J4-FO6-383652	1
Fagron	SyrSpend® SF Alka	18J25B15	1
Fagron	SyrSpend® SF Alka	18I25-B15-357803	1
Fagron	SyrSpend® SF Alka	19F06-B02_363789	1
Fargon	SyrSpend® SF Alka	21B26F07378133	1
Fagron	SyrSpend® SF Alka	19K07F04367548	1
Krieger	SyrSpend® SF Alka	22BO4-FO6-381564	1
Noweda	SyrSpend® SF Alka	22J04-FO6-383652	1
Fagron	SyrSpend® SF Alka	18h01b12353473	1
Phoenix	SyrSpend® SF Alka	19D29-B07-362182	22
Phoenix	SyrSpend® SF Alka	FO3-3788208	1
Phönix	SyrSpend® SF Alka	18B13-B11-350851	1
Phönix	SyrSpend® SF Alka	21F08-F03378828	1
Phönix	SyrSpend® SF Alka	22B04-F04-381555	10
Fagron	SyrSpend® SF Alka	18j25b15357803	1
Sanacorp	SyrSpend® SF Alka	21F08-F03-378828210166	1
Sanacorp	SyrSpend® SF Alka	22804-F07	1
Fagron	SyrSpend® SF Alka	18121-b11-359901	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	SyrSpend® SF pH4	22L20-F03-384076	3
	SyrSpend® SF pH4	F02-2845309	1
	SyrSpend® SF pH4	22I09-F01-283384	1
	SyrSpend® SF pH4	23B13-F02-3845309	1
	SyrSpend® SF pH4	23B13-F02-384539	2
	SyrSpend® SF pH4	22I09-F03-383490	3
	SyrSpend® SF pH4	23E23-F05-385116	1
	SyrSpend® SF pH4	23A03-F09-384187	1
	SyrSpend® SF pH4	22I09-F03	1
	SyrSpend® SF pH4	22k08-F02-93826	1
	SyrSpend® SF pH4	23E22-F03-384948	1
	SyrSpend® SF pH4	F05-3811006	1
Fagron	SyrSpend® SF pH4	16J10-B03	3
Bombastus	SyrSpend® SF pH4	18I16-B01-357703	1
Caelo	SyrSpend® SF pH4	18A22_B05_346147	1
Caelo	SyrSpend® SF pH4	20A09-F03-369540	8
Fagon/Novatis	SyrSpend® SF pH4	20F08-f03	1
Fagron	SyrSpend® SF pH4	19j10-f09-364007	1
Fagron	SyrSpend® SF pH4	20c24-F02-372398	1
Fagron	SyrSpend® SF pH4	15A26-B04-305667	1
Fagron	SyrSpend® SF pH4	16J10-B03-330757	12
Fagron	SyrSpend® SF pH4	16/10-B03	1
Fagron	SyrSpend® SF pH4	19A14-B07_362431	1
Fagron	SyrSpend® SF pH4	19J10-F09	5
Fagron	SyrSpend® SF pH4	F08-3669902	1
Fagron	SyrSpend® SF pH4	20C24-F09	1
Fagron	SyrSpend® SF pH4	20A09-F03	11
Fagron	SyrSpend® SF pH4	20A09-F03-3695400	1
Fagron	SyrSpend® SF pH4	20c24-F02	1
Fagron	SyrSpend® SF pH4	20C24-F02	2
Fagron	SyrSpend® SF pH4	21K22-F06	1
Fagron	SyrSpend® SF pH4	20c24-f02-372398	1
Fagron	SyrSpend® SF pH4	20F18-F13-379343	23
Fagron	SyrSpend® SF pH4	20F08-F03-0000	1
Fagron	SyrSpend® SF pH4	20F08-F04-372518	1
Fagron	SyrSpend® SF pH4	22G07-H08	1
Fagron	SyrSpend® SF pH4	20F18-F14	2
Fagron	SyrSpend® SF pH4	22C07-F04-0000	1
Fagron	SyrSpend® SF pH4	22C07-F04-382813	8
Fagron	SyrSpend® SF pH4	22C07-F04	1
Fagron	SyrSpend® SF pH4	F02-3834809	3
Fagron	SyrSpend® SF pH4	22I09-F03-383490	1
Fagron	SyrSpend® SF pH4	22109-F02	1
Fagron	SyrSpend® SF pH4	11111346	1
Fagron	SyrSpend® SF pH4	22K01-H01	1
Fagron	SyrSpend® SF pH4	22L20-F03-384076	1
Fagron	SyrSpend® SF pH4	23A03-F10-384538	2
Fagron	SyrSpend® SF pH4	18J16-B01	2
Fagron	SyrSpend® SF pH4	22C07-F03	2
Fagron	SyrSpend® SF pH4	F03-3725107	1
Fagron	SyrSpend® SF pH4	211021-01	1
Fagron	SyrSpend® SF pH4	21H20-F02-380674	9
Fagron	SyrSpend® SF pH4	22B04-F02381139	1
Fagron	SyrSpend® SF pH4	21L07-F05-381032	1
Fagron	SyrSpend® SF pH4	22K08-F02-383826	12
Fagron	SyrSpend® SF pH4	22I09-F02-383489	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF pH4	22I09-F01-383384	3
Fagron	SyrSpend® SF pH4	22I09-F01-383384	1
Fagron	SyrSpend® SF pH4	22K08F02-383826	1
Fagron	SyrSpend® SF pH4	18A22_B04_346147	1
Fagron	SyrSpend® SF pH4	19J10-F09-366992	1
Fagron	SyrSpend® SF pH4	16710-B03	1
Fagron	SyrSpend® SF pH4	18H30B02355226	1
Fagron	SyrSpend® SF pH4	20F08-F03-372517	19
Fagron	SyrSpend® SF pH4	20F08-F03	6
Fagron	SyrSpend® SF pH4	16J10B03330757	1
Fagron	SyrSpend® SF pH4	18/16-B01-357703	1
Fagron	SyrSpend® SF pH4	19j10F09	1
Fagron	SyrSpend® SF pH4	19L05-f10-368874	1
Fagron	SyrSpend® SF pH4	18A22-B05-346147	6
Fagron	SyrSpend® SF pH4	20F08_F03_372517	1
Fagron	SyrSpend® SF pH4	F03-3725107	1
Fagron	SyrSpend® SF pH4	22109-F03-383490	1
Fagron	SyrSpend® SF pH4	18H30-B02	9
Fagron	SyrSpend® SF pH4	18H30-355226	1
Fagron	SyrSpend® SF pH4	22C07-F03-382305	6
Fagron	SyrSpend® SF pH4	18J16_B01_357703	1
Fagron	SyrSpend® SF pH4	18H30_B02_355226	2
Fagron	SyrSpend® SF pH4	19J10-F08-366993	7
Fagron	SyrSpend® SF pH4	F08-3669903	2
Fagron	SyrSpend® SF pH4	19J10-F08-3669903	1
Fagron	SyrSpend® SF pH4	F09-3670004	1
Fagron	SyrSpend® SF pH4	18J16-B01-357703	15
Fagron	SyrSpend® SF pH4	19j10-f09-367004	2
Fagron	SyrSpend® SF pH4	F10-3688704	2
Fagron	SyrSpend® SF pH4	19J10-F08-366992	2
Fagron	SyrSpend® SF pH4	16J10_B03_330757	1
Fagron	SyrSpend® SF pH4	16j10-b03-330757	1
Fagron	SyrSpend® SF pH4	19J10-f08366993	1
Fagron	SyrSpend® SF pH4	19J10-FO8-366992	1
Fagron	SyrSpend® SF pH4	19j10-F09-367004	1
Fagron	SyrSpend® SF pH4	19j10-F08-366992	1
Fagron	SyrSpend® SF pH4	1BL21-B11	1
Fagron	SyrSpend® SF pH4	20C24-F02-372398	17
Fagron	SyrSpend® SF pH4	18H30-B02-355226	18
Fagron	SyrSpend® SF pH4	19A14-B07	3
Fagron	SyrSpend® SF pH4	F03-3695400	1
Fagron	SyrSpend® SF pH4	16J10B03	1
Fagron	SyrSpend® SF pH4	18J16B01357703	1
Fagron	SyrSpend® SF pH4	19J10-F09-367004	6
Fagron	SyrSpend® SF pH4	19/10-F09-367004	1
Fagron	SyrSpend® SF pH4	19L05-F10-368874	13
Fagron	SyrSpend® SF pH4	19L05-F1O-368874	1
Fagron	SyrSpend® SF pH4	20C24-F02	8
Fagron	SyrSpend® SF pH4	20F18-F14-379344	10
Fagron	SyrSpend® SF pH4	19L05-F10-3688704	1
Fagron	SyrSpend® SF pH4	F02-3723908	4
Fagron	SyrSpend® SF pH4	22C07F04382813	1
Fagron	SyrSpend® SF pH4	18A22-B05-347899	6
Fagron	SyrSpend® SF pH4	19L05-F10-368874	1
Fagron	SyrSpend® SF pH4	22J04-F06-383652	1
Gehe	SyrSpend® SF pH4	19A14-B07-362431	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF pH4	22007-F04	1
Kehr	SyrSpend® SF pH4	23E22-F01-384947	2
noweda	SyrSpend® SF pH4	15I22-B02-52176	1
Noweda	SyrSpend® SF pH4	2209-F03-383490	1
Fagron	SyrSpend® SF pH4	18A22-B05	2
Fagron	SyrSpend® SF pH4	19J10-F08	8
Noweda/Hedinger	SyrSpend® SF pH4	18J16-B01-357703	1
Phoenix	SyrSpend® SF pH4	18L21-B11-359901	1
Phoenix	SyrSpend® SF pH4	18J25-B15-357803	1
Fagron	SyrSpend® SF pH4	19L05-F10	5
Sanacorp	SyrSpend® SF pH4	23E22-F02-384949	1
	SyrSpend® SF pH4 neo	H09-0094001	1
Fagron	SyrSpend® SF pH4 neo	23J11-H01-00941	1
Fagron	SyrSpend® SF pH4 neo	24B28-H08-00941	1
Sanacorp	SyrSpend® SF pH4 neo	24H06-H07-00941	1

T

Supplier	Substance	Batch	Spectra
Caelo	Talco	11318324	4
Caelo	Talco	28121201	1
Caelo	Talco	11164313	1
Caelo	Talco	11164306	1
Caelo	Talco	12267401	4
Caelo	Talco	9218303	1
Caelo	Talco	12267412	7
Caelo	Talco	11318312	2
Caelo	Talco	15061301	1
Caelo	Talco	13146301	1
Caelo	Talco	13146308	6
Caelo	Talco	13146307	3
Caelo	Talco	13146312	4
Caelo	Talco	2011406	1
Caelo	Talco	13146316	3
Caelo	Talco	13146315	1
Caelo	Talco	12267424	5
Caelo	Talco	12267423	3
Caelo	Talco	11318311	3
Caelo	Talco	11318335	4
Caelo	Talco	13146302	8
Caelo	Talco	11318301	1
EuRho	Talco	1105024-02	1
Euro OTC	Talco	1205046-01	2
Euro OTC	Talco	1305022-01	7
Euro OTC	Talco	1210052-01	4
Euro OTC	Talco	1305022-02	1
Phönix	Talco	10148805Retest	1
Caelo	Talidomida	20081504	1
Fagron	Talidomida	14E27-B04-299297	1
Fagron	Talidomida	13K20-N01	1
Caelo	Tanaceto	12380204	1
Caelo	Tanaceto	12380203	5
Sanacorp	Tanaceto	12380201	2
Caelo	Tanchagem	14125907	1
Caelo	Tanchagem	10349610	1
Caelo	Tanchagem	12374104	7
Caelo	Tanchagem	123741004	1
Caelo	Tanchagem	10349614	1
Caelo	Tanchagem	12374106	2
Caelo	Tanchagem	13232401	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tanchagem	13232404	1
Caelo	Tanchagem	10349603	2
Caelo	Tanchagem	10349605	1
Caelo	Tanchagem	12374101	4
Caelo	Tanchagem	9311208	1
Klenk	Tanchagem	4281N110404	1
Klenk	Tanchagem	N111121	1
Klenk	Tanchagem	4281N111121	5
apomix	Tartarato de ergotamina	15L01-B02	1
Fagron	Tartarato de ergotamina	15B16-B05-308417	1
Fagron	Tartarato de ergotamina	15L01-B02-341852	1
Fagron	Tartarato de ergotamina	18D05-B01-358419	2
Fagron	Tartarato de ergotamina	18D05-B01-36779	1
Caelo	Tartarato de potássio hemi-...	11225007	1
Caelo	Tartarato de potássio hemi-...	27061304	1
Caelo	Tartarato de potássio hemi-...	12322110	1
Caelo	Tartarato de potássio hemi-...	13111415	1
Caelo	Tartarato de potássio hemi-...	13331113	1
Caelo	Tartarato de potássio hemi-...	15167703	1
Caelo	Tartarato de potássio hemi-...	24061705	1
Caelo	Tartarato de potássio hemi-...	17176002	2
Caelo	Tartarato de potássio hemi-...	19051804	1
Caelo	Tartarato de potássio hemi-...	17176004	1
Caelo	Tartarato de potássio hemi-...	17176007	1
Caelo	Tartarato de potássio hemi-...	18220301	2
Caelo	Tartarato de potássio hemi-...	193079002	1
Caelo	Tartarato de potássio hemi-...	193079004	1
Caelo	Tartarato de potássio hemi-...	18220305	2
Caelo	Tartarato de potássio hemi-...	17176001	2
Caelo	Tartarato de sódio e potáss...	15375601	12
Caelo	Tartarato de sódio e potáss...	17257701	4
Caelo	Teriaga	12289301	4
Caelo	Teriaga	11082413	1
Caelo	Teriaga	2021301	1
Caelo	Teriaga	15101307	1
Caelo	Teriaga	412091-2P	1
Caelo	Teriaga	12289312	1
Caelo	Teriaga	13407304	2
Caelo	Teriaga	15026401	3
Caelo	Teriaga	11081515	1
Caelo	Teriaga	15312501	2
Caelo	Teriaga	1531501	1
Caelo	Teriaga	15312511	2
Caelo	Teriaga	14156501	1
Caelo	Teriaga	12289307	8
Caelo	Teriaga	12189404	2
Caelo	Teriaga	12289305	2
Caelo	Teriaga	15312508	1
Caelo	Teriaga	12289303	1
Caelo	Teriaga	12289306	1
Caelo	Teriaga	15312504	1
Caelo	Teriaga	12189401	1
Caesar/Noweda	Teriaga	12289309	1
Klenk	Teriaga	12189403	1
Caelo	Tiosulfato de sódio pentahi...	80426288	1
Caelo	Tiosulfato de sódio pentahi...	26041302	1
Fagron	Tiosulfato de sódio pentahi...	13092013E	1
Fagron	Tiosulfato de sódio pentahi...	12F20-N20	1
Fagron	Tiosulfato de sódio pentahi...	12F20-N10	1
Fagron	Tiosulfato de sódio pentahi...	3313U-01922	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Aurica	Tomilho	521207003	1
Bahnhof-Apotheke	Tomilho	17-121112	1
Bombastus	Tomilho	277996	2
Bombastus	Tomilho	277466	1
Bombastus	Tomilho	243485	1
Caelo	Tomilho	10365807	2
Caelo	Tomilho	10365816	1
Caelo	Tomilho	8061206	1
Caelo	Tomilho	11345004	4
Caelo	Tomilho	15101201	1
Caelo	Tomilho	12111201	1
Caelo	Tomilho	11345007	5
Caelo	Tomilho	21121204	1
Caelo	Tomilho	11345001	1
Caelo	Tomilho	11345010	6
Caelo	Tomilho	29011303	1
Caelo	Tomilho	11021301	1
Caelo	Tomilho	22021301	1
Caelo	Tomilho	23021304	1
Caelo	Tomilho	26021301	1
Caelo	Tomilho	4041301	1
Caelo	Tomilho	11345014	12
Caelo	Tomilho	25041302	1
Caelo	Tomilho	11345013	9
Caelo	Tomilho	1134514	1
Caelo	Tomilho	13081301	1
Caelo	Tomilho	25091304	1
Caelo	Tomilho	29101301	1
Caelo	Tomilho	11121306	1
Caelo	Tomilho	13011402	1
Caelo	Tomilho	13048308	2
Caelo	Tomilho	16011401	1
Caelo	Tomilho	4021512	1
Caelo	Tomilho	13048314	1
Caelo	Tomilho	14119001	1
Caelo	Tomilho	15104401	1
Caelo	Tomilho	11345002	1
Caelo	Tomilho	11345006	3
Caelo	Tomilho	13048302	2
Caelo	Tomilho	13048301	14
Caelo	Tomilho	13048309	4
Caelo	Tomilho	10365815	2
Caelo	Tomilho	11345011	13
Caelo	Tomilho	13048309-3475312161	1
Euro OTC	Tomilho	4622A130109	75
Galke	Tomilho	19386	2
Galke	Tomilho	28719	1
Galke	Tomilho	20719	2
Galke	Tomilho	1833	1
Gehe	Tomilho	4622A110120	1
Klenk	Tomilho	4622A110728	25
Klenk	Tomilho	4622A120111	35
Hepart AG	Tomilho	A130109	2
Klenk	Tomilho	4622a110728	1
Klenk	Tomilho	1910211688	1
Klenk	Tomilho	4622a130109	2
Klenk	Tomilho	4622A141203	1
Klenk	Tomilho	4622B110519	1
Klenk	Tomilho	2103311688	1
Klenk	Tomilho	A130910	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Tomilho	4622A130910	2
Klenk	Tomilho	4622A12011	1
Klenk	Tomilho	4622A-120111	1
Klenk	Tomilho	4622A170207	1
Klenk	Tomilho	4622A170905	3
Klenk	Tomilho	4622a120111	3
Noweda	Tomilho	521303908	1
Bombastus	Tomilho	273909	3
Caelo	Tomilho		1
Weltecke	Tomilho	67101212	1
-	Tomilho selvagem, cortada	131023	1
-	Tomilho selvagem, cortada	130685	1
Caelo	Tomilho selvagem, cortada	11031203	1
Caelo	Tomilho selvagem, cortada	11374805	5
Caelo	Tomilho selvagem, cortada	11374805i.O.	1
Caelo	Tomilho selvagem, cortada	4501A120813	2
Caelo	Tomilho selvagem, cortada	13086805	3
Caelo	Tomilho selvagem, cortada	11374803	1
Caesar & Loretz Gm...	Tomilho selvagem, cortada	11374802	1
Finze	Tomilho selvagem, cortada	11031204	1
Gehe	Tomilho selvagem, cortada	1090413	1
vedono	Tomilho selvagem, cortada	11374807	2
Aurica	Tormentilha	521304332	1
Caelo	Tormentilha	11102010	1
Caelo	Tormentilha	12040704	2
Caelo	Tormentilha	10081203	1
Caelo	Tormentilha	2512A-02188	1
Caelo	Tormentilha	12040717	1
Caelo	Tormentilha	12216802	1
Caelo	Tormentilha	12040707	1
Caelo	Tormentilha	411082-2-P	1
Caelo	Tormentilha	30011405	1
Caelo	Tormentilha	25022014A	1
Caelo	Tormentilha	14008005	1
Caelo	Tormentilha	15085501	1
Caelo	Tormentilha	14360103	1
Caelo	Tormentilha	15178203	1
Caelo	Tormentilha	15178206	1
Caelo	Tormentilha	15364316	1
Caelo	Tormentilha	12216806	1
Caelo	Tormentilha	14008001	2
Caelo	Tormentilha	15364302	5
Caelo	Tormentilha	4753268	1
Caelo	Tormentilha	12040708	9
Caelo	Tormentilha	12040713	1
Caelo	Tormentilha	1914A-02188	1
Caelo	Tormentilha	6911B140227	1
Caelo	Tormentilha	14140001	1
Caelo	Tormentilha	15178202	2
Caelo	Tormentilha	12216803	4
Caelo	Tormentilha	12216805	1
Caelo	Tormentilha	14008002	2
Caelo	Tormentilha	12216801	4
Cealo/Gehe	Tormentilha	14140006	3
Galke	Tormentilha	21091	1
Galke	Tormentilha	21744	2
Caelo	Tormentilha	13220502	1
Klenk	Tormentilha	6911B131029	4
Klenk	Tormentilha	6911B141114	2
Klenk	Tormentilha	6911B150825	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Tormentilha	6911B140227	1
Klenk	Tormentilha	6911B111013	10
Klenk	Tormentilha	6914b120112	1
kräuter schulte	Tormentilha	51952	1
Noweda10.02.2017	Tormentilha	15364313	3
phönix	Tormentilha	15364343	1
Phönix	Tormentilha	15364302	1
Richter	Tormentilha	P209904	1
Sanacorp	Tormentilha	12040712	3
AHD	Tragacanto	15379906	5
Caelo	Tragacanto	8081201	1
Caelo	Tragacanto	9081202	1
Caelo	Tragacanto	15121203	1
Caelo	Tragacanto	11128905	1
Caelo	Tragacanto	12285402	1
Caelo	Tragacanto	14011302	1
Caelo	Tragacanto	12285403	4
Caelo	Tragacanto	1228503	1
Caelo	Tragacanto	15041302	1
Caelo	Tragacanto	13095203	1
Caelo	Tragacanto	13095208	3
Caelo	Tragacanto	20111305	1
Caelo	Tragacanto	7021402	1
Caelo	Tragacanto	13277802	4
Caelo	Tragacanto	14162205	7
Caelo	Tragacanto	13204705	1
Caelo	Tragacanto	15085607	1
Caelo	Tragacanto	153799	1
Caelo	Tragacanto	16110802	2
Caelo	Tragacanto	14162207	1
Caelo	Tragacanto	15379907	1
Caelo	Tragacanto	14162207	2
Caelo	Tragacanto	13204701	4
Caelo	Tragacanto	15085606	7
Caelo	Tragacanto	13277804	4
Caelo	Tragacanto	15085602	1
Caelo	Tragacanto	12108806	1
Caelo	Tragacanto	1327802	1
Caelo	Tragacanto	12285408	1
Caelo	Tragacanto	16110807	3
Caelo	Tragacanto	16350004	1
Fagron	Tragacanto	13204705	5
JENNE	Tragacanto	16110801	1
Caelo	Tragacanto	15085602	4
Fagron	Triancinolona acetonida 1:1…	12107-N04	1
Fagron	Triancinolona acetonida 1:1…	11g14-n02	1
Fagron	Triancinolona acetonida 1:1…	11G14-N02	1
Fagron	Triancinolona acetonida 1:1…	13F21-N01	2
Fagron	Triancinolona acetonida 1:1…	12F21-N01	1
Fagron	Triancinolona acetonida 1:1…	14F17-N02	1
Fagron	Triancinolona acetonida 1:1…	13A15-N05	1
Fagron	Triancinolona acetonida 1:1…	13F20-N010113/150	1
Fagron	Triancinolona acetonida 1:1…	12107-N04022/359	1
Fagron	Triancinolona acetonida 1:1…	12I07-No4	1
Fagron	Triancinolona acetonida 1:1…	12G23-N06	2
Fagron	Triancinolona acetonida 1:1…	12I07-N04	1
Fargon/17.07.2013/…	Triancinolona acetonida 1:1…	12|07-N04	1
Fagron	Triancinolona acetonida 1:1…	12A05-N07	3
Fagron	Triancinolona acetonida 1:1…	12E23-N01	2
Bombastus	Tussilago farfara, folha	277848	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Tussilago farfara, folha	269501	3
Bombastus	Tussilago farfara, folha	272019	1
Bombastus	Tussilago farfara, folha	276303	5
Bombastus	Tussilago farfara, folha	285263	3
Bombastus	Tussilago farfara, folha	265856	1
Bombastus	Tussilago farfara, folha	274289	5
Bombastus	Tussilago farfara, folha	275489	3
Bombastus	Tussilago farfara, folha	281100	4
Bombastus	Tussilago farfara, folha	277131	1
Bombastus	Tussilago farfara, folha	232339	1
Bombastus	Tussilago farfara, folha	278758	7
Caelo	Tussilago farfara, folha	23041302	1
Caelo	Tussilago farfara, folha	Int.Ch:Now16081	1
Gehe	Tussilago farfara, folha	2021B121204	9
Klenk	Tussilago farfara, folha	8061207	1
Klenk	Tussilago farfara, folha	11101202	1
Klenk	Tussilago farfara, folha	2021B120124	4
Klenk	Tussilago farfara, folha	2021B120601	5
Klenk	Tussilago farfara, folha	5011301	1
Klenk	Tussilago farfara, folha	20021301	1
Klenk	Tussilago farfara, folha	KS100061	1
Klenk	Tussilago farfara, folha	2021B130319	4
Klenk	Tussilago farfara, folha	B120124	1
Klenk	Tussilago farfara, folha	26091301	1
Klenk	Tussilago farfara, folha	14111302	1
Klenk	Tussilago farfara, folha	5122013a	1
Klenk	Tussilago farfara, folha	23121302	1
Klenk	Tussilago farfara, folha	B130227	1
Klenk	Tussilago farfara, folha	2021C140730	1
Klenk	Tussilago farfara, folha	2021B150407	1
Klenk	Tussilago farfara, folha	2020B120124	1
Klenk	Tussilago farfara, folha	2021B130227	12
Klenk	Tussilago farfara, folha	2021B111005	1
Klenk	Tussilago farfara, folha	2021B140131	1
Klenk	Tussilago farfara, folha	2021b121204	1
Klenk	Tussilago farfara, folha	2021C130326	8
Noweda	Tussilago farfara, folha	2021B111111	3
Phönix	Tussilago farfara, folha	278296	4
Klenk	Tussilago farfara, folha	2021B121203	5

U

Supplier	Substance	Batch	Spectra
Audor Pharma	Uridina	AP721060040/5U	3
Audor Pharma	Uridina	AP3015	1
Audor Pharma	Uridina	APIB1600182AU	8
Audor Pharma	Uridina	APIB1600169AU	44
Audor Pharma	Uridina	APIB1600169	2
Audor Pharma	Uridina	APIB1600169AU/Re	1
Audor Pharma	Uridina	AP30514U	5
Audor Pharma	Uridina	APIB1400280AU	1
Audor Pharma	Uridina	APIB1600182.11AU	1
Audor Pharma	Uridina	APIB16001169	1
Audor Pharma	Uridina	AP30514IB1500001AXU	5
Audor Pharma	Uridina	IB1600169AU	3
Caelo	Uridina	AP1600169AU	1
Caelo	Uridina	IB1600169A	1
Fagron	Uridina	11G07-N04	1
Fagron	Uridina	22041301	1
Fagron	Uridina	16101301	1
Fagron	Uridina	14051405	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Uridina	13D08-N26	1
Fagron	Uridina	721110090	4
Fagron	Uridina	12091402	1
Fagron	Uridina	APIB16000169au	1
Fagron	Uridina	13K18-B31	4
Fagron	Uridina	14F02-B09	1
Fagron	Uridina	13D29-N06	3
Fagron	Uridina	14F02-B09-305467	7
Phönix	Uridina	721010040	1
Roth / Roth	Uridina	410301476	1
siehe WE-Prüfprotokoll	Uridina	54/11	1
Caelo	Urtiga, raiz	10081202	1
Caelo	Urtiga, raiz	11254902	3
Caelo	Urtiga, raiz	11254903	5
Caelo	Urtiga, raiz	11265002	5
Caelo	Urtiga, raiz	11265003	2
Caelo	Urtiga, raiz	6631B130610	1
Caelo	Urtiga, raiz	11265006	1
Caelo	Urtiga, raiz	11265004	4
Caelo	Urtiga, raiz	11254904	3
Gehe	Urtiga, raiz	6631B120927	5
Caelo	Urtiga, raiz	6441A121024	1
Klenk	Urtiga, raiz	6631N110513	1
Klenk	Urtiga, raiz	6631B120416	1
Klenk	Urtiga, raiz	9931B120927	1
Sanacorp	Urtiga, raiz	11265001	2
Alliance	Urze, cortada	255389	1
Bombastus	Urze, cortada	278314	1
Caelo	Urze, cortada	28061201	1
Caelo	Urze, cortada	9291512	1
Caelo	Urze, cortada	19111203	1
Caelo	Urze, cortada	11011209	3
Caelo	Urze, cortada	11102901	1
Caelo	Urze, cortada	13367502	1
Caesar/Noweda	Urze, cortada	4911I-03224	1
Nachprüfung	Urze, cortada	5110A03224	1

V

Supplier	Substance	Batch	Spectra
Klenk	Valeriana, raiz cortada	6641B120417	1
Aurica	Valeriana, raiz cortada	221838	2
Bombastus	Valeriana, raiz cortada	267863	1
Bombastus	Valeriana, raiz cortada	274722	1
Bombastus	Valeriana, raiz cortada	269457	1
Caelo	Valeriana, raiz cortada	12033812	8
Caelo	Valeriana, raiz cortada	11103601	1
Caelo	Valeriana, raiz cortada	11103602	1
Caelo	Valeriana, raiz cortada	11103608	1
Caelo	Valeriana, raiz cortada	11349101	4
Caelo	Valeriana, raiz cortada	11103612	2
Caelo	Valeriana, raiz cortada	3091202	1
Caelo	Valeriana, raiz cortada	11035002	1
Caelo	Valeriana, raiz cortada	31101202	1
Caelo	Valeriana, raiz cortada	11103607	3
Caelo	Valeriana, raiz cortada	31121201	1
Caelo	Valeriana, raiz cortada	12033805	4
Caelo	Valeriana, raiz cortada	2712A-02167	1
Caelo	Valeriana, raiz cortada	12033809	9
Caelo	Valeriana, raiz cortada	1203381	1
Caelo	Valeriana, raiz cortada	20081303	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Valeriana, raiz cortada	12033810	1
Caelo	Valeriana, raiz cortada	120338012	1
Caelo	Valeriana, raiz cortada	28101303	1
Caelo	Valeriana, raiz cortada	29101303	1
Caelo	Valeriana, raiz cortada	13287402	3
Caelo	Valeriana, raiz cortada	15175205	1
Caelo	Valeriana, raiz cortada	12033811	5
Caelo	Valeriana, raiz cortada	11103609	4
Caelo	Valeriana, raiz cortada	12033807	1
Caelo	Valeriana, raiz cortada	13119001	1
Caelo	Valeriana, raiz cortada	13119004	3
Caelo	Valeriana, raiz cortada	13119003	12
Caelo	Valeriana, raiz cortada	13196806	6
Caelo	Valeriana, raiz cortada	13196801-3564412081	1
Caelo	Valeriana, raiz cortada	13196802	4
Galke	Valeriana, raiz cortada	22070	1
Galke	Valeriana, raiz cortada	21798	4
Klenk	Valeriana, raiz cortada	13196808	1
Klenk	Valeriana, raiz cortada	6641B110317	2
Klenk	Valeriana, raiz cortada	6641B-110317	1
Klenk	Valeriana, raiz cortada	6641B100823	1
Klenk	Valeriana, raiz cortada	6645B130226	1
Klenk	Valeriana, raiz cortada	6641B130226	9
Caelo	Valeriana, raiz cortada	13119002	18
Caelo	Valeriana, raiz cortada	1319003	1
Sanacorp	Valeriana, raiz cortada	12033804	9
Caelo	Valeriana, raiz cortada	12033808	7
Caelo	Vara-de-ouro (Solidago virg…	12343103	17
Anzag 17.04.13 ek:…	Vara-de-ouro (Solidago virg…	4521A110816	2
Aurica	Vara-de-ouro (Solidago virg…	521201267	1
Aurica	Vara-de-ouro (Solidago virg…	224133	1
Bomba/AHD	Vara-de-ouro (Solidago virg…	279526	1
Bombastus	Vara-de-ouro (Solidago virg…	261756	1
Bombastus	Vara-de-ouro (Solidago virg…	271459	1
Bombastus	Vara-de-ouro (Solidago virg…	270047	2
Bombastus	Vara-de-ouro (Solidago virg…	271460	1
Bombastus	Vara-de-ouro (Solidago virg…	278697	2
Bombastus	Vara-de-ouro (Solidago virg…	209974	1
Caelo	Vara-de-ouro (Solidago virg…	314050-1-p	1
Caelo	Vara-de-ouro (Solidago virg…	11207010	3
Caelo	Vara-de-ouro (Solidago virg…	15061203	1
Caelo	Vara-de-ouro (Solidago virg…	265283	1
Caelo	Vara-de-ouro (Solidago virg…	11280301	4
Caelo	Vara-de-ouro (Solidago virg…	17091203	1
Caelo	Vara-de-ouro (Solidago virg…	11280308	9
Caelo	Vara-de-ouro (Solidago virg…	20111209	1
Caelo	Vara-de-ouro (Solidago virg…	112080308	1
Caelo	Vara-de-ouro (Solidago virg…	12319002	2
Caelo	Vara-de-ouro (Solidago virg…	28051302	1
Caelo	Vara-de-ouro (Solidago virg…	6081302	1
Caelo	Vara-de-ouro (Solidago virg…	12343104	5
Caelo	Vara-de-ouro (Solidago virg…	4091302	1
Caelo	Vara-de-ouro (Solidago virg…	12343102	3
Caelo	Vara-de-ouro (Solidago virg…	14112012	1
Caelo	Vara-de-ouro (Solidago virg…	27121302	1
Caelo	Vara-de-ouro (Solidago virg…	4021405	1
Caelo	Vara-de-ouro (Solidago virg…	12343109	1
Caelo	Vara-de-ouro (Solidago virg…	13386903	1
Caelo	Vara-de-ouro (Solidago virg…	13386901	1
Caelo	Vara-de-ouro (Solidago virg…	14018404	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Vara-de-ouro (Solidago virg…	2656153	1
Caelo	Vara-de-ouro (Solidago virg…	12343105	1
Caelo	Vara-de-ouro (Solidago virg…	11280309	1
Caelo	Vara-de-ouro (Solidago virg…	12336801	1
Caelo	Vara-de-ouro (Solidago virg…	12319007	21
Caelo	Vara-de-ouro (Solidago virg…	12319006	3
Caelo	Vara-de-ouro (Solidago virg…	12319004	10
Caelo	Vara-de-ouro (Solidago virg…	4113A-01684	1
Caelo	Vara-de-ouro (Solidago virg…	11280310	6
Caelo	Vara-de-ouro (Solidago virg…	12343106	1
Caesar & Loretz Gm…	Vara-de-ouro (Solidago virg…	11207014	3
Galke	Vara-de-ouro (Solidago virg…	21079	2
Gehe	Vara-de-ouro (Solidago virg…	11207011	1
Gehe	Vara-de-ouro (Solidago virg…	11280311	2
Caelo	Vara-de-ouro (Solidago virg…	12343101	3
Klenk	Vara-de-ouro (Solidago virg…	A110209	1
Klenk	Vara-de-ouro (Solidago virg…	4521A-110816	1
Klenk	Vara-de-ouro (Solidago virg…	4521A100414	1
Klenk	Vara-de-ouro (Solidago virg…	4521A110209	4
Noweda	Vara-de-ouro (Solidago virg…	11280306	3
Caelo	Vara-de-ouro (Solidago virg…	12319003	22
Bombastus	Vara-de-ouro (Solidago virg…	274290	1
an	Verbena	12383007	1
Aurica	Verbena	521305668	1
Caelo	Verbena	11031106	5
Caelo	Verbena	11031108	5
Caelo	Verbena	11031103	1
Caelo	Verbena	11031110	6
Caelo	Verbena	19111205	1
Caelo	Verbena	12187601	15
Caelo	Verbena	12178601	1
Caelo	Verbena	12188203	6
Caelo	Verbena	4651b120611	1
Caelo	Verbena	13151001	18
Caelo	Verbena	12383002	2
Caelo	Verbena	6111301	1
Caelo	Verbena	12383005	1
Caelo	Verbena	13351401	1
Caelo	Verbena	15012405	1
Caelo	Verbena	11031105	2
Caelo	Verbena	12188202	14
Caelo	Verbena	2x12188202	1
Caelo	Verbena	13151003	5
Gehe	Verbena	4651B110310	2
Klenk	Verbena	4651A070828	3
Klenk	Verbena	4654B120611	1
Klenk	Verbena	A130923	1
Klenk	Verbena	4651B130611	2
Klenk	Verbena	4651B120611	17
Caelo	Verbena	110031110	1
A.H. 27.05.13 ek: 6,75EUR	Veronica officinalis	274239	1
Anzag ek: 4,88EUR 26…	Veronica officinalis	4661C120321	10
Aurica/Phönix	Veronica officinalis	520708362	1
Bahnhof-Apotheke	Veronica officinalis	4-121002	1
Bombastus	Veronica officinalis	274238	1
Caelo	Veronica officinalis	12162503	1
Caelo	Veronica officinalis	11265503	5
Caelo	Veronica officinalis	11265502	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Veronica officinalis	4661c111011	1
Caelo	Veronica officinalis	3051306	1
Caelo	Veronica officinalis	12162504	13
Caelo	Veronica officinalis	11061305	1
Caelo	Veronica officinalis	28061303	1
Caelo	Veronica officinalis	3091305	1
Caelo	Veronica officinalis	13166701	3
Caelo	Veronica officinalis	14111303	1
Caelo	Veronica officinalis	20111303	1
Caelo	Veronica officinalis	1216504	1
Caelo	Veronica officinalis	12162505	2
Finze	Veronica officinalis	4661B080915	1
Klenk	Veronica officinalis	4661A090318	1
Klenk	Veronica officinalis	4661B110916	1
Klenk	Veronica officinalis	4661C120802	13
Klenk	Veronica officinalis	4661C130226	27
Klenk	Veronica officinalis	C120321	1
Klenk	Veronica officinalis	C130226	5
Klenk	Veronica officinalis	4661C13026	1
Klenk	Veronica officinalis	4661C131104	1
Klenk	Veronica officinalis	4661C111011	13
Klenk	Veronica officinalis	4661B101011	1
Klenk	Veronica officinalis	4661C130226-32743106	1
Klenk	Veronica officinalis	4661c130226-34343111	1
Klenk	Veronica officinalis	4661C2004	1
Klenk	Veronica officinalis	4661C-111011	1
Klenk	Veronica officinalis	4661B110121	2
Klenk	Veronica officinalis	6661C130226	1
Klenk	Veronica officinalis	4661c120802	1
Klenk	Veronica officinalis	4661c120321	1
Phönix	Veronica officinalis	13089201	4
Bombastus	Viola tricolor, erva	276259	3
Bombastus	Viola tricolor, erva	280890	1
Bombastus	Viola tricolor, erva	274237	2
Bombastus	Viola tricolor, erva	272832	1
Bombastus	Viola tricolor, erva	278106	2
Bombastus	Viola tricolor, erva	279314	3
Bombastus	Viola tricolor, erva	282661	2
Bombastus	Viola tricolor, erva	278106	2
Bombastus	Viola tricolor, erva	220232	1
Caelo	Viola tricolor, erva	10291007	1
Caelo	Viola tricolor, erva	13091205	1
Caelo	Viola tricolor, erva	10291009	3
Caelo	Viola tricolor, erva	17101205	1
Caelo	Viola tricolor, erva	5021304	1
Caelo	Viola tricolor, erva	15021301	1
Caelo	Viola tricolor, erva	11216103	2
Caelo	Viola tricolor, erva	12189203	4
Caelo	Viola tricolor, erva	14061311	1
Caelo	Viola tricolor, erva	7101303	1
Caelo	Viola tricolor, erva	12382806	1
Caelo	Viola tricolor, erva	12189204	4
Caelo	Viola tricolor, erva	12189204	10
Caelo	Viola tricolor, erva	4681A180411	1
Caelo	Viola tricolor, erva	12189204-3458312120	1
Caelo	Viola tricolor, erva	1289203	1
Caelo	Viola tricolor, erva	12189203	5
Caelo	Viola tricolor, erva	12382802	1
Caelo	Viola tricolor, erva	12189204-3463312101	1
Fagron	Viola tricolor, erva		1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Viola tricolor, erva	11216103	3
Klenk	Viola tricolor, erva	4681A110303	2
Klenk	Viola tricolor, erva	4681A120806	1
Klenk	Viola tricolor, erva	B130715	1
Klenk	Viola tricolor, erva	4681B130715	5
Klenk	Viola tricolor, erva	4681A181105	1
Klenk	Viola tricolor, erva	4681A-120806	1
Klenk	Viola tricolor, erva	4681A120806	15
Nachprüfung	Viola tricolor, erva	10291007	1
Sanacorp	Viola tricolor, erva	12221-01694	1
Caelo	Violeta, cortada	11124008	1
Caelo	Violeta, cortada	13038701	4
Caelo	Violeta, cortada	11124007	1
Caelo	Violeta, cortada	1303872	1
Caelo	Violeta, cortada	13038703	2
Caelo	Violeta, cortada	10011403	1
Caelo	Violeta, cortada	13232107	1
Caelo	Violeta, cortada	11124007-3284310662	1
Anzag ek:2,64EUR 16.07.12	Visco	10273417	1
Aurica/Phönix	Visco	6110801	1
Bombastus	Visco	277432	2
Caelo	Visco	29061201	1
Caelo	Visco	10273412	1
Caelo	Visco	10081205	1
Caelo	Visco	10091201	1
Caelo	Visco	11294003	2
Caelo	Visco	23111204	1
Caelo	Visco	10273418	1
Caelo	Visco	10273420	5
Caelo	Visco	12011301	1
Caelo	Visco	11266704	14
Caelo	Visco	11021303	1
Caelo	Visco	11266708	8
Caelo	Visco	11266705	3
Caelo	Visco	18031303	1
Caelo	Visco	11266710	7
Caelo	Visco	6061306	1
Caelo	Visco	17061304	1
Caelo	Visco	26071302	1
Caelo	Visco	29071302	1
Caelo	Visco	29081302	1
Caelo	Visco	28101304	1
Caelo	Visco	29101302	1
Caelo	Visco	20121303	1
Caelo	Visco	27121305	1
Caelo	Visco	24011401	1
Caelo	Visco	14292506	2
Caelo	Visco	14292514	1
Caelo	Visco	11266714	4
Caelo	Visco	11266703	3
Caelo	Visco	11266712-3450311162	1
Caelo	Visco	11266702	4
Caelo	Visco	10273407	1
Caelo	Visco	11294004	5
Caelo	Visco	3813E-01695	1
Caelo	Visco	4313E-01695	1
Caelo	Visco	11266713	2
Galke	Visco	20328	1
Galke	Visco	22012	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gesundform	Visco	216482	1
Haustee	Visco	57010507	1
Caelo	Visco	11294005	15
Klenk	Visco	4691A120507	2
Klenk	Visco	4691A110816	2
Klenk	Visco	1512211695	1
Klenk	Visco	2901311695	1
Klenk	Visco	110816	1
Klenk	Visco	4691A130307	7
Klenk	Visco	4691A121122	11
Klenk	Visco	4961A120419	1
Klenk	Visco	4691a130307	1
Klenk	Visco	4691A-120507	1
Klenk	Visco	4691a121122	1
Klenk	Visco	4691A121122-35454110	1
Noweda	Visco	11294001	1
Caelo	Visco	11266709	10
Caelo	Visco	11266712	8
Klenk	Visco	4691A120419	6
Spangropharm	Visco	10273408	1

Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

> *"Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features."*

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

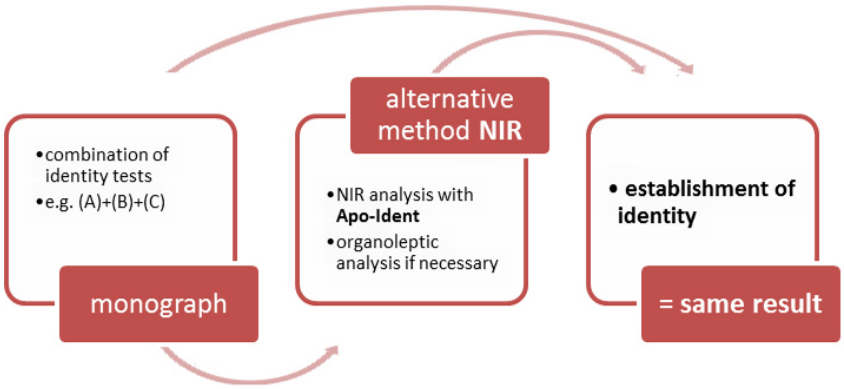


Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

Appendix E: Conformity of *Apo-Ident* with the *European pharmacopeia*

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: "Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials" ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of "Meeting *2.2.40 Ph. Eur.* by *Apo-Ident*" [4].

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Appendix F: Addition to the second-stage models

As described in the general part of the *Apo-Ident* validation documentation, in the section Model creation procedure and validation runs, under *2. Generating the chemometric models (calibration)* in *f)*, it is possible to create a further chemometric model for certain substances (second-stage model) and to undertake the assessment in several steps.

Substances in second-stage models

In the substance class *BR IFAs e excipientes sólidos*, a distinction is made between the following substances in the listed second-stage models:

Submodell - Submodelo 01

Base para supositório (Witepsol W35)
Cera de abelha, amarela
Cera de abelha, branca
Dodecilsulfato de sódio
Estearato de magnésio
Gordura sólida
Manteiga de cacau
Palmitato de cetila
Parafina sólida
Parafina, microcristalina

Submodell - Submodelo 02

Betametasona
Dexametasona
Fluocinolona acetonida
Gramicidina
Metilprednisolona
Prednisolona
Tirotricina
Triancinolona acetonido

Submodell - Submodelo 03

Ácido oxálico
Amido de arroz
Amido de milho
Amido de trigo
Anfotericina B
Bacitracina
Bromidrato de hioscina
Carmelose sódica
Cianocobalamina
Concentrado seco de colecalciferol
Estradiol hemi-hidratado
Estriol
Fécula de batata
Folha de eucalipto
Frutose
Gelatina, branca
Glicerofosfato de cálcio
Goma arábica, dispersão seca

Lactobionato de eritromicina
Levedura de selênio
Maltodextrina
Metilcobalamina
Nistatina
Pantotenato de cálcio
Riboflavina
Sulfato de colistina
Sulfato de polimixina B
SyrSpend® SF Alka
SyrSpend® SF pH4
SyrSpend® SF pH4 neo
Tosilcloramida sódica
Triancinolona
Vitamina E acetato pó 50%

Submodell - Submodelo 04

Carbômero
Citrato de magnésio
Finasterida
Fosfato de Mg-Ca-K-colamina
Fosfato sódico de riboflavina hidratado
Gluconato de zinco
Sulfato de gentamicina
Sulfato de neomicina
Sulfato de tobramicina
Tetraborato de sódio

Submodell - Submodelo 05

Ácido fusídico
Espironolactona
Iodopovidona
Povidona
Progesterona
Propionato de testosterona
Ubidecarenona

Submodell - Submodelo 07

Budesonida
Eritromicina
Valerato de betametasona

Submodell - Submodelo 08

Acetato de prednisolona
Cloridrato de efedrina
Prednisona

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Submodell - Submodelo 09

Ácido acetilsalicílico
Ácido benzoico
Cloreto de dequalínio
Cloridrato de oxitetraciclina
Ditranol
Eosina amarela
Levotiroxina sódica
Salicilato de sódio
Tanino

Submodell - Submodelo 12

Ácido nicotínico
Clioquinol
Mesalazina
Nitrato de miconazol
Teofilina etilenodiamina hidratada

Submodell - Submodelo 13

Acetato de ciproterona
Acetato de noretisterona
Alfaestradiol
Amifampridina
Capsaicina
Citrato de sódio
Cloridrato de amitriptilina
Cloridrato de ciprofloxacina
Cloridrato de oxibutinina
Cloridrato de quinina di-hidratado
Heparina sódica
Levocarnitina
Metoxisaleno
Piridoxal-5-fosfato
Prednicarbato
Sacarose
Tetracaína
Triclosan
Valina

Submodell - Submodelo 14

Citrato monobásico de magnésio, hidratado
Cloridrato de propranolol
Escina, hidrossolúvel
Fenitoína
Furoato de mometasona
Hidrocortisona
Orotato de cálcio di-hidratado
Quinolina amarela
Sacarina sódica
Sorbato de potássio

Sulfato de atropina

Submodell - Submodelo 15

Dipropionato de beclometasona
Dipropionato de betametasona
Propionato de clobetasol

Submodell - Submodelo 18

Benzoato de sódio
Difenilciclopropenona

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

References

[1] ABDA – Bundesvereinigung Deutscher Apothekerverbände: Verordnung über den Betrieb von Apotheken (Apothekenbetriebsordnung – ApBetrO), 2012

[2] Reimann, B. ; Regierungspräsidium Darmstadt: Hinweise zur ordnungsgemäßen Prüfung von Arzneimitteln und Ausgangsstoffen (§§ 6 und 11 *ApBetrO*), 2007

[3] *Europäisches Arzneibuch, Implementation 2022*. 11. Edition. Deutscher Apotheker Verlag (978-3-7692-8026-5)

[4] HiperScan GmbH: Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident, 2013

[5] Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD): Resolution in Verbindung mit §§ 6 und 11 *ApBetrO* Verwendung eines Nah-Infrarot-Spektrometers (NIR) zur Identitätsprüfung, 16. 10. 2013, DAZ 48, November 2013

[6] Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD): Resolution 2014, Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD), Oktober 2014

[7] *DAC/NRF*. Govi-Verlag (978-3-7741-0044-2)

[8] Kessler, W.: *Multivariate Datenanalyse*. WILEY-VCH Verlag, 2007 (978-3-527-31262-7)

[9] Næs, T. ; Isaksson, T. ; Fearn, T. ; Davies, T.: *Multivariate Calibration and Classification*. NIR Publications, 2002 (978 0 9528666 2 6)

[10] Hanley, J. A. ; Lippman-Hand, A.: If nothing goes wrong, is everything all right? In: *Journal of the American Medical Association* 249 (1983), S. 1743–1745

[11] Jovanovic, B. D. ; Levy, P. S.: A Look at the Rule of Three. In: *The American Statistician* 51 (1997), S. 137–139

[12] Bronstein, I. N. ; Semendjajew, K. A. ; Musiol, G. ; Mühlig, H.: *Taschenbuch der Mathematik*. 5. überarbeitete und erweiterte Auflage. Verlag Harri Deutsch, 2000 (3-8171-2015-2)

[13] Mahalanobis, P.: On the generalized distance in statistics. In: *Proc. Nat. Inst. Sci. India (Calcutta)* 2 (1936), S. 49–55

[14] Yambor, B. ; Draper, W. ; Beveridge, R.: Analyzing PCA-based face recognition algorithms: Eigenvector selection and distance measures. In: *Second Workshop Empirical Evaluation in Computer Vision* (2000)

[15] HiperScan GmbH: Identifikationsmethodik Apo-Ident, 2012

[16] HiperScan GmbH: Datenvorbehandlung des Identifikationssystems Apo-Ident, 2012

[17] Cyran ; Rotta: Apothekenbetriebsordnung, Kommentar § 6 Rn. 10, 2010

Index

4-hidroxibenzoato de metila, 25
4-hidroxibenzoato de propila, 33

Acaciae gummi dispersione desiccatum, *see* Goma arábica, dispersão seca, 1785
Acetato de ciproterona, 39
Acetato de dexametasona, 47
Acetato de hidrocortisona, 55
Acetato de noretisterona, 81
Acetato de prednisolona, 89
Acetato de Racealfatocoferol 50%, *see* Concentrado seco de acetato de alfa-tocoferol, 1299
Acetato de sódio tri-hidratado, 109
Acetato de zinco di-hidratado, 115
Acetilcisteína, 121
Aciclovir, 127
Aciclovirum, *see* Aciclovir, 127
Acidum 4-aminobenzoicum, *see* Ácido 4-aminobenzoico, 133
Acidum acetylsalicylicum, *see* Ácido acetilsalicílico, 137
Acidum aminolaevulinicum hydrochloricum, *see* Cloridrato do ácido 5-aminolevulínico, 1245
Acidum asparticum, *see* Ácido aspártico, 153
Acidum benzoicum, *see* Ácido benzoico, 157
Acidum boricum, *see* Ácido bórico, 163
Acidum citricum, *see* Ácido cítrico, 169
Acidum citricum monohydricum, *see* Ácido cítrico monoidratado, 193
Acidum folicum hydricum, *see* Ácido fólico hidratado, 207
Acidum fusidicum, *see* Ácido fusídico, 213
Acidum glutaminicum, *see* Ácido glutâmico, 219
Acidum nicotinicum, *see* Ácido nicotínico, 225
Acidum oxalicum cryst., *see* Ácido oxálico, 231
Acidum salicylicum, *see* Ácido salicílico, 237
Acidum sorbicum, *see* Ácido sórbico, 261
Acidum stearicum, *see* Ácido esteárico 50, 201
Acidum tartaricum, *see* Ácido tartárico, 269
Acidum tranexamicum, *see* Ácido tranexâmico, 279
Adeps solidus, *see* Ceras/gorduras, 633
Adeps solidus W35, *see* Ceras/gorduras, 633
Adrenalini tartras, *see* Hemitartarato de epinefrina, 1827
Aescinum solubile, *see* Escina, hidrossolúvel, 1497
Alanina levógira, *see* L-alanina, 1989
Alaninum, *see* L-alanina, 1989
Alantoína, 291
Albendazol, 299
Albendazolum, *see* Albendazol, 299
Alcohol cetylicus, *see* Álcool cetoestearílico, 311
Alcohol cetylicus et stearylicus, *see* Álcool cetoestearílico, 311
Alcoholes emulsificantes nonionici, *see* Álcool emulsificante não iônico, 327
Alcoholes lanae, *see* Álcoois de cera de lã, 305
Alfa-tocoferol acetato 50%, *see* Concentrado seco de acetato de alfa-tocoferol, 1299
Alfaestradiol, 333
Alfatradiolum, *see* Alfaestradiol, 333
Allantoinum, *see* Alantoína, 291
Allopurinolum, *see* Alopurinol, 345
Alopurinol, 345
Aluminii chloridum hexahydricum, *see* Cloreto de alumínio hexa-hidratado, 827
Ambroxol, cloridrato, *see* Cloridrato de ambroxol, 861
Ambroxoli hydrochloridum, *see* Cloridrato de ambroxol, 861
Amfetamini sulfas, *see* Sulfato de anfetamina, 2675
Amido, 351
Amido de arroz, *see* Amido, 351
Amido de milho, *see* Amido, 351
Amido de trigo, *see* Amido, 351
Amifampridina, 369
Amifampridinum, *see* Amifampridina, 369
Amilorida, cloridrato di-hidratado, *see* Cloridrato de amilorida di-hidratado, 873
Amiloridi hydrochloridum dihydricum, *see* Cloridrato de amilorida di-hidratado, 873
Amitriptilina, cloridrato, *see* Cloridrato de amitriptilina, 879
Amitriptylini hydrochloridum, *see* Cloridrato de amitriptilina, 879
Amlodipini besilas, *see* Besilato de anlodipino, 471
Ammonii hydrogencarbonas, *see* Bicarbonato de amônio, 485
Amoxicilina tri-hidratada, 375
Amoxicillinum trihydricum, *see* Amoxicilina tri-hidratada, 375
Amphotericinum B, *see* Anfotericina B, 381
Amylum Maydis, *see* Amido, 351
Amylum oryzae, *see* Amido, 351
Anfetamina, sulfato, *see* Sulfato de anfetamina, 2675

Anfotericina B, 381
Anlodipino, besilato, *see* Besilato de anlodipino, 471
Antralina, *see* Ditranol, 1425
Argentum proteinicum, *see* Proteinato de prata, 2573
Arginina, 387
Arginina, cloridrato, *see* Cloridrato de arginina, 887
Argininum, *see* Arginina, 387
Ascorbato de cálcio di-hidratado, 393
Ascorbato de sódio, 399
Ascorbylis palmitas, *see* Palmitato de ascorbila, 2381
Aspartato de ornitina, 405
Aspartato monobásico de magnésio tetra-hidratado, 411
Atropina, sulfato, *see* Sulfato de atropina, 2683
Atropini sulfas, *see* Sulfato de atropina, 2683
Azul patente V, 417

Bacitracina, 423
Bacitracinum, *see* Bacitracina, 423
Baclofeno, 431
Baclofenum, *see* Baclofeno, 431
Barbital sódico, 437
Barbitalum natricum, *see* Barbital sódico, 437
Base para supositório (Witepsol W35), *see* Ceras/gorduras, 633
Beclometasona, dipropionato, *see* Dipropionato de beclometasona, 1405
Beclometasoni dipropionas, *see* Dipropionato de beclometasona, 1405
Benzidamina, cloridrato, *see* Cloridrato de benzidamina, 893
Benzoato de estradiol, 441
Benzoato de sódio, 451
Benzocainum, *see* Benzocaína, 461
Benzocaína, 461
Benzydamini hydrochloridum, *see* Cloridrato de benzidamina, 893
Besilato de anlodipino, 471
Betainum monohydricum, *see* Betaína monoidratada, 475
Betametasona, 479
Betametasona, dipropionato, *see* Dipropionato de betametasona, 1411
Betamethasoni dipropionas, *see* Dipropionato de betametasona, 1411
Betamethasoni valeras, *see* Valerato de betametasona, 3041
Betamethasonum, *see* Betametasona, 479
Betametosona, valerato, *see* Valerato de betametasona, 3041
Betaína monoidratada, 475
BHT, *see* Hidroxitolueno butilado, 1907
Bicarbonato de amônio, 485
Bifonazol, 491
Bifonazolum, *see* Bifonazol, 491
Biotina, 497
Biotinum, *see* Biotina, 497
Bismuthi subgallas, *see* Galato de bismuto, básico, 1689
Bitartarato de potássio, 503
Borax, *see* Tetraborato de sódio, 2853
Brometo de butilescopolamina, 509
Brometo de glicopirrônio, 515
Brometo de ipratrópio, 521
Brometo de neostigmina, 527
Bromidrato de dextrometorfano, 533
Bromidrato de hioscina, 539
Bromidrato de homatropina, 545
Budesonida, 549
Budesonidum, *see* Budesonida, 549
Bupivacaini hydrochloridum, *see* Cloridrato de bupivacaína, 901
Bupivacaína, cloridrato, *see* Cloridrato de bupivacaína, 901
Butilbrometo de escopolamina, *see* Brometo de butilescopolamina, 509
Butilescopolamina, brometo, *see* Brometo de butilescopolamina, 509
Butilhidroxitolueno, *see* Hidroxitolueno butilado, 1907
Butylhydroxytoluenum, *see* Hidroxitolueno butilado, 1907
Bórax, *see* Tetraborato de sódio, 2853

Cafeína, 559
Calcii ascorbas dihydricum, *see* Ascorbato de cálcio di-hidratado, 393
Calcii gluconas, *see* Gluconato de cálcio, 1755
Calcii glycerophosphas, *see* Glicerofosfato de cálcio, 1707
Calcii hydrogenphosphas dihydricus, *see* Fosfato de cálcio monobásico di-hidratado, 1597
Calcii lactas pentahydricus, *see* Lactato de cálcio penta-hidratado, 1957
Calcii pantothenas, *see* Pantotenato de cálcio, 2395
Camphora racemica, *see* Cânfora racêmica/cânfora D, 583
Canabidiol, 567
Capsacinum, *see* Capsaicina, 591
Capsaicina, 591
Captopril, 597
Captoprilum, *see* Captopril, 597
Carbomera, *see* Carbômero, 607
Carboximetilcelulose sódica, *see* Carmelose sódica, 619
Carbômero, 607

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Carmellosum natricum, *see* Carmelose sódica, 619
Carmelose sódica, 619
Carnitina levógira, *see* Levocarnitina, 2011
Cellulosum microcristallinum, *see* Celulose microcristalina, 627
Celulose microcristalina, 627
Cera alba, *see* Ceras/gorduras, 633
Cera de abelha, amarela, *see* Ceras/gorduras, 633
Cera de abelha, branca, *see* Ceras/gorduras, 633
Cera flava, *see* Ceras/gorduras, 633
Ceras/gorduras, 633
Cetamina, cloridrato, *see* Cloridrato de cetamina, 905
Cetearyl Alcohol (and) Ceteareth-20 (base autoemulsionável não-iônica), *see* Álcool cetoestearílico, 311
Cetoconazol, 669
Cetostearyl alcohol (type A), emulsifying, *see* Álcool cetoestearílico, 311
Cetylis palmitas, *see* Ceras/gorduras, 633
Chinidini sulfas, *see* Sulfato de quinidina di-hidratado, 2757
Chinini hydrochloridum dihydricum, *see* Cloridrato de quinina di-hidratado, 1191
Chinini sulfas, *see* Sulfato de quinina, 2763
Chlorali hydras, *see* Hidrato de cloral, 1845
Chloramphenicolum, *see* Cloranfenicol, 809
Chlorhexidini acetas, *see* Diacetato de clorexidina, 1333
Chlorocresolum, *see* Clorocresol, 1251
Chlorprothixeni hydrochloridum, *see* Cloridrato de clorprotixeno, 953
Chlortetracyclini hydrochloridum, *see* Cloridrato de clortetraciclina, 957
Cholesterolum, *see* Colesterol, 1291
Cholinii chloridum, *see* Cloreto de colina, 835
Cholinium bitartaricum, *see* Hemifumarato de colina, 1809
Cianocobalamina, *see* Cianocobalamina/Metilcobalamina, 677
Cianocobalamina/Metilcobalamina, 677
Ciclamato de sódio, 683
Ciclopirox olamina, 689
Ciclopirox olaminum, *see* Ciclopirox olamina, 689
Ciclosporina, 697
Ciclosporinum, *see* Ciclosporina, 697
Ciproeptadina, cloridrato hidratado, *see* Cloridrato de cipro-heptadina 1,5-hidrato, 917
Ciprofloxacina, cloridrato, *see* Cloridrato de ciprofloxacina, 911
Ciprofloxacini hydrochloridum, *see* Cloridrato de ciprofloxacina, 911
Ciproterona, acetato, *see* Acetato de ciproterona, 39
Cistina, 705
Citrato de cafeína, 711
Citrato de cálcio tetra-hidratado, 717
Citrato de fentanila, 725
Citrato de magnésio, 731
Citrato de potássio, 737
Citrato de potássio monoidratado, *see* Citrato de potássio, 737
Citrato de sildenafila, 747
Citrato de sódio, 757
Citrato monobásico de magnésio, hidratado, 775
Citrulina, 787
Citrullinum, *see* Citrulina, 787
Clindamicina, cloridrato, *see* Cloridrato de clindamicina, 927
Clindamycini hydrochloridum, *see* Cloridrato de clindamicina, 927
Clindamycini phosphas, *see* Fosfato dibásico de clindamicina 2, 1609
Clioquinol, 793
Clioquinolum, *see* Clioquinol, 793
Clobetasol, propionato, *see* Propionato de clobetasol, 2537
Clobetasoli propionas, *see* Propionato de clobetasol, 2537
Clonidina, cloridrato, *see* Cloridrato de clonidina, 941
Clonidini hydrochloridum, *see* Cloridrato de clonidina, 941
Cloranfenicol, 809
Cloreto de alumínio hexa-hidratado, 827
Cloreto de colina, 835
Cloreto de dequalínio, 839
Cloreto de magnésio hexa-hidratado, 849
Cloreto de metacolina, 855
Clorexidina, diacetato, *see* Diacetato de clorexidina, 1333
Cloridrato de ambroxol, 861
Cloridrato de amilorida di-hidratado, 873
Cloridrato de amitriptilina, 879
Cloridrato de arginina, 887
Cloridrato de benzidamina, 893
Cloridrato de bupivacaína, 901
Cloridrato de cetamina, 905
Cloridrato de cipro-heptadina 1,5-hidrato, 917
Cloridrato de ciproeptadina hidratado, *see* Cloridrato de cipro-heptadina 1,5-hidrato, 917
Cloridrato de ciprofloxacina, 911
Cloridrato de cisteína monoidratado, 921
Cloridrato de clindamicina, 927
Cloridrato de clonidina, 941

Cloridrato de cloreto de tiamina, 947
Cloridrato de clorprotixeno, 953
Cloridrato de clortetraciclina, 957
Cloridrato de cocaína, 965
Cloridrato de difenidramina, 971
Cloridrato de diltiazem, 977
Cloridrato de doxepina, 1001
Cloridrato de efedrina, 1007
Cloridrato de fenilefrina, 1013
Cloridrato de hidromorfona, 1019
Cloridrato de isoxsuprina, 1025
Cloridrato de lidocaína monoidratado, 1029
Cloridrato de lisina, 1049
Cloridrato de mepivacaína, 1055
Cloridrato de metadona, 1061
Cloridrato de metoclopramida monoidratado, 1075
Cloridrato de midazolam, 1081
Cloridrato de morfina, 1087
Cloridrato de nafazolina, 1095
Cloridrato de naloxona di-hidratado, 1103
Cloridrato de naltrexona, 1109
Cloridrato de noscapina monoidratado, 1113
Cloridrato de ornitina, 1117
Cloridrato de oxibuprocaína, 1123
Cloridrato de oxibutinina, 1129
Cloridrato de oxitetraciclina, 1137
Cloridrato de papaverina, 1147
Cloridrato de pilocarpina, 1153
Cloridrato de piridoxina, 1159
Cloridrato de prilocaína, 1165
Cloridrato de procaína, 1171
Cloridrato de propranolol, 1179
Cloridrato de quinina di-hidratado, 1191
Cloridrato de ropivacaína monoidratado, 1197
Cloridrato de sotalol, 1201
Cloridrato de tetracaína, 1205
Cloridrato de tetraciclina, 1221
Cloridrato de vancomicina, 1231
Cloridrato de xilometazolina, 1237
Cloridrato do ácido 5-aminolevulínico, 1245
Cloridrato do ácido aminolevulínico, *see* Cloridrato do ácido 5-aminolevulínico, 1245
Clorocresol, 1251
Clorprotixeno, cloridrato, *see* Cloridrato de clorprotixeno, 953
Clortetraciclina, cloridrato, *see* Cloridrato de clortetraciclina, 957
Clotrimazol, 1257
Clotrimazolum, *see* Clotrimazol, 1257
CMC-Na, *see* Carmelose sódica, 619
Cocaini hydrochloridum, *see* Cloridrato de cocaína, 965
Cocaína, cloridrato, *see* Cloridrato de cocaína, 965
Codeini phosphas hemihydricus, *see* Fosfato de codeína hemi-hidratado, 1603
Coenzima Q10, *see* Ubidecarenona, 3007
Coffeini citras, *see* Citrato de cafeína, 711
Coffeinum, *see* Cafeína, 559
Colesterol, 1291
Colina, cloreto, *see* Cloreto de colina, 835
Colina, hemifumarato, *see* Hemifumarato de colina, 1809
Colistina, sulfato, *see* Sulfato de colistina, 2689
Colistini sulfas, *see* Sulfato de colistina, 2689
Concentrado seco de acetato de alfa-tocoferol, 1299
Cromoglicato de sódio, 1305
Curcumina, 1311
Cyanocobalaminum, *see* Cianocobalamina/Metilcobalamina, 677
Cyproheptadini hydrochloridum-1,5-hydricum, *see* Cloridrato de cipro-heptadina 1,5-hidrato, 917
Cyproteroni acetas, *see* Acetato de ciproterona, 39
Cysteini hydrochloridum monohydricum, *see* Cloridrato de cisteína monoidratado, 921
Cânfora D, *see* Cânfora racêmica/cânfora D, 583
Cânfora racêmica, *see* Cânfora racêmica/cânfora D, 583
Cânfora racêmica/cânfora D, 583

D-Camphora, *see* Cânfora racêmica/cânfora D, 583
Dehidroepiandrosterona, *see* Prasterona, 2435
Dequalinii chloridum, *see* Cloreto de dequalínio, 839
Dexametasona, 1315
Dexametasona, acetato, *see* Acetato de dexametasona, 47
Dexamethasoni acetas, *see* Acetato de dexametasona, 47
Dexamethasonum, *see* Dexametasona, 1315
Dexamfetamini sulfas, *see* Sulfato de dexanfetamina, 2699
Dexanfetamina, sulfato, *see* Sulfato de dexanfetamina, 2699
Dextromethorphani hydrobromidum monohydricum, *see* Bromidrato de dextrometorfano, 533
Dextrometorfano bromidrato, *see* Bromidrato de dextrometorfano, 533
DHEA, *see* Prasterona, 2435
Di-hidrocodeína, tartarato, *see* Di-hidrocodeína[(R,R)-tartarato],

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

1379
Di-hidrocodeína[(R,R)-tartarato], 1379
Diacetato de clorexidina, 1333
Diclofenaco sódico, 1343
Diclofenacum natricum, *see* Diclofenaco sódico, 1343
Dicloridrato de histamina, 1353
Dicloridrato de octenidina, 1359
Difenciprona, *see* Difenilciclopropenona, 1373
Difenidramina, cloridrato, *see* Cloridrato de difenidramina, 971
Difenilciclopropenona, 1373
Dihidrogenofosfato de potássio, 1385
Dihydrocodeini hydrogenotartras, *see* Di-hidrocodeína[(R,R)-tartarato], 1379
Diltiazem, cloridrato, *see* Cloridrato de diltiazem, 977
Diltiazemi hydrochloridum, *see* Cloridrato de diltiazem, 977
Dinatrii edetas, *see* Edetato de sódio, 1439
Dinitrato de isossorbida 40%, 1389
Diosmina, 1401
Diphenhydramini hydrochloridum, *see* Cloridrato de difenidramina, 971
Diphenylcyclopropenonum, *see* Difenilciclopropenona, 1373
Dipirona sódica monoidratada, *see* Metamizol sódico monoidratado, 2159
Dipropionato de beclometasona, 1405
Dipropionato de betametasona, 1411
Dithranolum, *see* Ditranol, 1425
Ditranol, 1425
DL metionina, 1435
DL-alfa-tocoferol acetato 50%, *see* Concentrado seco de acetato de alfa-tocoferol, 1299
DL-Methioninum, *see* DL metionina, 1435
Dodecilsulfato de sódio, *see* Ceras/gorduras, 633
Doxepina, cloridrato, *see* Cloridrato de doxepina, 1001
Doxepini hydrochloridum, *see* Cloridrato de doxepina, 1001
Doxiciclina, hiclato, *see* Hiclato de doxiciclina, 1839
Doxycyclini hyclas, *see* Hiclato de doxiciclina, 1839
Doxylamini hydrogenosuccinas, *see* Hemissuccinato de doxilamina, 1815

Edetato de sódio, 1439
Edetato dissódico de cálcio, 1451
EDTA dissódico, *see* Edetato de sódio, 1439
EDTA dissódico de cálcio, *see* Edetato dissódico de cálcio, 1451
Efedrina, cloridrato, *see* Cloridrato de efedrina, 1007
Emulgade® 1000 NI, *see* Álcool cetoestearílico, 311
Enalapril, maleato, *see* Maleato de enalapril, 2077
Enalaprili maleas, *see* Maleato de enalapril, 2077
Eosina amarela, 1457
Eosina amarelada, *see* Eosina amarela, 1457
Eosina Y, *see* Eosina amarela, 1457
Eosinum natricum, *see* Eosina amarela, 1457
Ephedrini hydrochloridum, *see* Cloridrato de efedrina, 1007
Epinefrina, hemitartarato, *see* Hemitartarato de epinefrina, 1827
Eritromicina, 1463
Erythromycinum, *see* Eritromicina, 1463
Escina, hidrossolúvel, 1497
Escopolamina, butilbrometo, *see* Brometo de butilescopolamina, 509
Espironolactona, 1503
Estearato de magnésio, 1515
Estearato de zinco, 1521
Estradiol hemi-hidratado, 1525
Estradiol, valerato, *see* Valerato de estradiol, 3071
Estradioli benzoas, *see* Benzoato de estradiol, 441
Estradioli valeras, *see* Valerato de estradiol, 3071
Estradiolum hemihydricum, *see* Estradiol hemi-hidratado, 1525
Estriol, 1535
Estriolum, *see* Estriol, 1535
Ethacridini lactas monohydricus, *see* Lactato de etacridina monoidratado, 1963
Ethinylestradiolum, *see* Etinilestradiol, 1545
Ethosuximidum, *see* Etossuximida, 1551
Etinilestradiol, 1545
Etossuximida, 1551

Fampridina, 1555
Fampridinum, *see* Fampridina, 1555
Fenazona, 1561
Fenilalanina levógira, *see* L-fenilalanina, 2023
Fenilbutazona, 1567
Fenilefrina, cloridrato, *see* Cloridrato de fenilefrina, 1013
Feniramina, maleato, *see* Maleato de feniramina, 2083
Fenitoína, 1573
Fenobarbital, 1579
Fentanila, citrato, *see* Citrato de fentanila, 725
Fentanyli citras, *see* Citrato de fentanila, 725

Ferrosi gluconas hydricus, *see* Gluconato ferroso hidratado, 1769
Finasterida, 1585
Finasteridum, *see* Finasterida, 1585
Fluocinolona acetonida, 1591
Fluocinoloni acetonidum, *see* Fluocinolona acetonida, 1591
Fosfato de codeína hemi-hidratado, 1603
Fosfato de cálcio monobásico di-hidratado, 1597
Fosfato de potássio dibásico, *see* Dihidrogenofosfato de potássio, 1385
Fosfato dibásico de clindamicina 2, 1609
Fosfato dibásico de sódio di-hidratado, 1615
Fosfato dissódico de prednisolona, 1621
Fosfato sódico de riboflavina hidratado, 1629
Fructosum, *see* Frutose, 1635
Frutose, 1635
Fumarato de quetiapina, 1649
Furoato de mometasona, 1653
Furosemida, 1673
Furosemidum, *see* Furosemida, 1673
Fécula de batata, *see* Amido, 351

Gabapentina, 1679
Gabapentinum, *see* Gabapentina, 1679
Galactose, 1683
Galactosum, *see* Galactose, 1683
Galato de bismuto, básico, 1689
Gelatina, branca, 1701
Gentamicina, sulfato, *see* Sulfato de gentamicina, 2705
Gentamicini sulfas, *see* Sulfato de gentamicina, 2705
Glicerofosfato de cálcio, 1707
Glicina, 1715
Glicinato de cálcio, *see* Gluconato de cálcio, 1755
Glicinato de zinco, *see* Gluconato de zinco, 1763
Glicinato ferroso hidratado, *see* Gluconato ferroso hidratado, 1769
Glicopirrônio, brometo, *see* Brometo de glicopirrônio, 515
Glicose, 1721
Glicose monoidratada, 1733
Gluconato de cálcio, 1755
Gluconato de zinco, 1763
Gluconato ferroso hidratado, 1769
Glucosum, *see* Glicose, 1721
Glucosum monohydricum, *see* Glicose monoidratada, 1733
Glutamina, 1773
Glutaminum, *see* Glutamina, 1773
Glutationa, 1779
Glyceroli monostearas 40–55, *see* Monoestearatos, 2257
Glyceroli monostearates 60, *see* Monoestearatos, 2257
Glyceroli monostearates emulsificantes, *see* Monoestearatos, 2257
Glycinum, *see* Glicina, 1715
Glycopyrronii bromidum, *see* Brometo de glicopirrônio, 515
Goma arábica, dispersão seca, 1785
Gordura sólida, *see* Ceras/gorduras, 633
Gramicidina, 1791
Gramicidinum, *see* Gramicidina, 1791
Griseofulvina, 1797
Griseofulvinum, *see* Griseofulvina, 1797
Guaifenesina, 1803
Guaifenesinum, *see* Guaifenesina, 1803

Hard fat W35, *see* Ceras/gorduras, 633
Hemifumarato de colina, 1809
Hemissuccinato de doxilamina, 1815
Hemissuccinato de prednisolona, 1821
Hemitartarato de epinefrina, 1827
Heparina sódica, 1833
Heparinum natricum, *see* Heparina sódica, 1833
Hiclato de doxiciclina, 1839
Hidrato de cloral, 1845
Hidrocarbonato de potássio, 1855
Hidroclorotiazida, 1861
Hidrocortisona, 1869
Hidrocortisona, acetato, *see* Acetato de hidrocortisona, 55
Hidromorfona, cloridrat, *see* Cloridrato de hidromorfona, 1019
Hidroquinona, 1893
Hidroxietilcelulose, 1901
Hidroxipropilcelulose, *see* Metilcelulose, 2165
Hidroxitolueno butilado, 1907
Hioscina, bromidrato, *see* Bromidrato de hioscina, 539
Hipromelose, *see* Metilcelulose, 2165
Histamina, dicloridrato, *see* Dicloridrato de histamina, 1353
Histamini dihydrochloridum, *see* Dicloridrato de histamina, 1353
Histidina, 1915
Histidinum, *see* Histidina, 1915
Homatropini hydrobromidum, *see* Bromidrato de homatropina, 545
Homotropina, bromidrato, *see* Bromidrato de homatropina, 545
HPMC, *see* Metilcelulose, 2165
Hydrochinonum, *see* Hidroquinona, 1893
Hydrochlorothiazidum, *see* Hidroclorotiazida, 1861
Hydrocortisoni acetas, *see* Acetato de hidrocortisona, 55
Hydrocortisonum, *see* Hidrocortisona, 1869

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Hydromorphoni hydrochloridum, *see* Cloridrato de hidromorfona, 1019
Hydroxyethylcellulosum, *see* Hidroxietilcelulose, 1901
Hydroxypropylcellulosum, *see* Metilcelulose, 2165
Hyoscini butylbromidum, *see* Brometo de butilescopolamina, 509

Ibuprofeno, 1921
Ibuprofenum, *see* Ibuprofeno, 1921
Indometacina, 1927
Indometacinum, *see* Indometacina, 1927
Iodoformium, *see* Iodofórmio, 1933
Iodofórmio, 1933
Iodopovidona, 1943
Ipratropii bromidum, *see* Brometo de ipratrópio, 521
Ipratrópio, brometo, *see* Brometo de ipratrópio, 521
Isoleucina, 1951
Isoleucinum, *see* Isoleucina, 1951
Isorbidi dinitras 40%, *see* Dinitrato de isossorbida 40%, 1389
Isossorbida, dinitrato 40%, *see* Dinitrato de isossorbida 40%, 1389
Isoxsuprina, cloridrato, *see* Cloridrato de isoxsuprina, 1025
Isoxsuprini hydrochloridum, *see* Cloridrato de isoxsuprina, 1025

Kalii dihydrogenophosphas, *see* Dihidrogenofosfato de potássio, 1385
Kalii hydrogencarbonas, *see* Hidrocarbonato de potássio, 1855
Kalii hydrogentartras, *see* Bitartarato de potássio, 503
Kalii sorbas, *see* Sorbato de potássio, 2641
Ketamini hydrochloridum, *see* Cloridrato de cetamina, 905

L-alanina, 1989
L-carnitina, *see* Levocarnitina, 2011
L-Carnitina Tartarato, *see* Tartarato de L-Carnitina, 2817
L-fenilalanina, 2023
L-treonina, 2045
Lactato de cálcio penta-hidratado, 1957
Lactato de etacridina monoidratado, 1963
Lactose monoidratada, 1971
Lactosum monohydricum, *see* Lactose monoidratada, 1971
Lauril sulfato de sódio, *see* Ceras/gorduras, 633
Lecithinum e sojae plv., *see* Lecitina de soja (forma instantânea), 1993
Lecitina de soja (forma instantânea), 1993
Leucina, 1999
Leucinum, *see* Leucina, 1999
Levedura de selênio, 2005
Levoalanina, *see* L-alanina, 1989
Levocarnitina, 2011
Levocarnitina Tartarato, *see* Tartarato de L-Carnitina, 2817
Levothyroxinum natrii, *see* Levotiroxina sódica, 2017
Levotiroxina sódica, 2017
Lidocaini hydrochloridum monohydricum, *see* Cloridrato de lidocaína monoidratado, 1029
Lidocainum, *see* Lidocaína, 2029
Lidocaína, 2029
Lidocaína, cloridrato monoidratado, *see* Cloridrato de lidocaína monoidratado, 1029
Lisina, cloridrato, *see* Cloridrato de lisina, 1049
Lithii orotas monohydricum, *see* Orotato de lítio monoidratado, 2353
Lysini hydrochloridum, *see* Cloridrato de lisina, 1049

Macrogol 1500, 2051
Macrogol 4000, 2057
Macrogolum 1500, *see* Macrogol 1500, 2051
Magnesii aspartas tetrahydricus, *see* Aspartato monobásico de magnésio tetra-hidratado, 411
Magnesii chloridum hexahydricum, *see* Cloreto de magnésio hexa-hidratado, 849
Magnesii citras, *see* Citrato de magnésio, 731
Magnesii hydrogenocitras hydricus, *see* Citrato monobásico de magnésio, hidratado, 775
Magnesii orotas dihydricus, *see* Orotato de magnésio di-hidratado, 2359
Magnesii stearas, *see* Estearato de magnésio, 1515
Magnesii sulfas heptahydricus, *see* Sulfato de magnésio hepta-hidratado, 2727
Maleato de enalapril, 2077
Maleato de feniramina, 2083
Maltodextrina, 2089
Maltodextrinum, *see* Maltodextrina, 2089
Mangani sulfas monohydricus, *see* Sulfato de manganês monoidratado, 2733
Manitol, 2095
Mannitolum, *see* Manitol, 2095
Manteiga de cacau, *see* Ceras/gorduras, 633
Melatonina, 2121
Melatoninum, *see* Melatonina, 2121
Mentholum, *see* Mentol, 2135
Mentol, 2135

Mepivacaini hydrochloridum, *see* Cloridrato de mepivacaína, 1055
Mepivacaína, cloridrato, *see* Cloridrato de mepivacaína, 1055
Mesalazina, 2153
Mesalazinum, *see* Mesalazina, 2153
Metadona, cloridrato, *see* Cloridrato de metadona, 1061
Metamizol sódico monoidratado, 2159
Methacholinii chloridum, *see* Cloreto de metacolina, 855
Methadoni hydrochloridum, *see* Cloridrato de metadona, 1061
Methoxsalenum, *see* Metoxisaleno, 2189
Methylcellulosum, *see* Metilcelulose, 2165
Methylis parahydroxybenzoas, *see* 4-hidroxibenzoato de metila, 25
Methylprednisolonum, *see* Metilprednisolona, 2177
Metilcelulose, 2165
Metilcobalamina, *see* Cianocobalamina/Metilcobalamina, 677
Metilprednisolona, 2177
Metionina, 2183
Metionina (DL), *see* DL metionina, 1435
Metoclopramida, cloridrato monoidratado, *see* Cloridrato de metoclopramida monoidratado, 1075
Metoclopramidi hydrochloridum monohydricum, *see* Cloridrato de metoclopramida monoidratado, 1075
Metoprolol, tartarato, *see* Tartarato de metoprolol, 2821
Metoprololi tartras, *see* Tartarato de metoprolol, 2821
Metoxisaleno, 2189
Metronidazol, 2199
Metronidazolum, *see* Metronidazol, 2199
Miconazol, nitrato, *see* Nitrato de miconazol, 2303
Miconazoli nitras, *see* Nitrato de miconazol, 2303
Midazolam, cloridrato, *see* Cloridrato de midazolam, 1081
Midazolami hydrochloridum, *see* Cloridrato de midazolam, 1081
Minoxidil, 2227
Minoxidil sulfate, *see* Minoxidil sulfato, 2249
Minoxidil sulfato, 2249
Minoxidilum, *see* Minoxidil, 2227
Mio-inositol, 2253
Mometasona, furoato, *see* Furoato de mometasona, 1653
Mometasoni furoas, *see* Furoato de mometasona, 1653
Monoestearato de glicerila 40-55, *see* Monoestearatos, 2257
Monoestearato de glicerila 60, *see* Monoestearatos, 2257
Monoestearato de glicerila emulsificante, *see* Monoestearatos, 2257
Monoestearato de glicerol 40-55, *see* Monoestearatos, 2257
Monoestearato de glicerol 60, *see* Monoestearatos, 2257
Monoestearato de glicerol, emulsionante, *see* Monoestearatos, 2257
Monoestearato de sorbitano, *see* Monoestearatos, 2257
Monoestearatos, 2257
Morfina, cloridrato, *see* Cloridrato de morfina, 1087
Morphini hydrochloridum, *see* Cloridrato de morfina, 1087
Mupirocina cálcica, 2267
Mupirocinum calcicum, *see* Mupirocina cálcica, 2267
myo-Inositolum, *see* Mio-inositol, 2253

N-acetilcisteína, *see* Acetilcisteína, 121
Nafazolina, cloridrato, *see* Cloridrato de nafazolina, 1095
Nafazolina, nitrato, *see* Nitrato de nafazolina, 2323
Naloxona, cloridrato di-hidratado, *see* Cloridrato de naloxona di-hidratado, 1103
Naloxoni hydrochloridum dihydricum, *see* Cloridrato de naloxona di-hidratado, 1103
Naltrexona, cloridrato, *see* Cloridrato de naltrexona, 1109
Naltrexoni hydrochloridum, *see* Cloridrato de naltrexona, 1109
Naphazolini hydrochloridum, *see* Cloridrato de nafazolina, 1095
Naphazolini nitras, *see* Nitrato de nafazolina, 2323
Naproxeno, 2273
Naproxenum, *see* Naproxeno, 2273
Natrii acetas trihydricum, *see* Acetato de sódio tri-hidratado, 109
Natrii ascorbas, *see* Ascorbato de sódio, 399
Natrii benzoas, *see* Benzoato de sódio, 451
Natrii calcii edetas, *see* Edetato dissódico de cálcio, 1451
Natrii citras, *see* Citrato de sódio, 757
Natrii cromoglicas, *see* Cromoglicato de sódio, 1305
Natrii cyclamas, *see* Ciclamato de sódio, 683
Natrii dihydrogenophosphas dihydricus, *see* Fosfato dibásico de sódio di-hidratado, 1615

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Natrii laurilsulfas, *see* Ceras/gorduras, 633
Natrii salicylas, *see* Salicilato de sódio, 2629
Natrii sulfas decahydricus, *see* Sulfato de sódio deca-hidratado, 2773
Neomicina, sulfato, *see* Sulfato de neomicina, 2737
Neomycini sulfas, *see* Sulfato de neomicina, 2737
Neostigmina, brometo, *see* Brometo de neostigmina, 527
Neostigmini bromidum, *see* Brometo de neostigmina, 527
Niacina, *see* Ácido nicotínico, 225
Nicotinamida, 2277
Nicotinamidum, *see* Nicotinamida, 2277
Nifedipina, 2283
Nifedipinum, *see* Nifedipina, 2283
Nistatina, 2287
Nitrato de miconazol, 2303
Nitrato de nafazolina, 2323
Nitrofurantoinum, *see* Nitrofurantoína, 2329
Nitrofurantoína, 2329
Norestisterona, acetato, *see* Acetato de noretisterona, 81
Norethisteroni acetas, *see* Acetato de noretisterona, 81
Noscapina, cloridrato monoidratado, *see* Cloridrato de noscapina monoidratado, 1113
Noscapini hydrochloridum hydricum, *see* Cloridrato de noscapina monoidratado, 1113

Octenidina, dicloridrato, *see* Dicloridrato de octenidina, 1359
Octenidini dihydrochloridum, *see* Dicloridrato de octenidina, 1359
Ofloxacino, 2335
Ofloxacinum, *see* Ofloxacino, 2335
Omeprazol, 2341
Omeprazolum, *see* Omeprazol, 2341
Orlistate, 2349
Ornithini aspartas, *see* Aspartato de ornitina, 405
Ornithini hydrochloridum, *see* Cloridrato de ornitina, 1117
Ornitina aspartato, *see* Aspartato de ornitina, 405
Ornitina, cloridrato, *see* Cloridrato de ornitina, 1117
Orotato de lítio monoidratado, 2353
Orotato de magnésio di-hidratado, 2359
Orotato de manganês di-hidratado, 2365
Orotato de zinco di-hidratado, 2371
Oxetacainum, *see* Oxetacaína, 2375
Oxetacaína, 2375
Oxibuprocaína, cloridrato, *see* Cloridrato de oxibuprocaína, 1123
Oxibutinina, cloridrato, *see* Cloridrato de oxibutinina, 1129
Oxitetraciclina, cloridrato, *see* Cloridrato de oxitetraciclina, 1137
Oxybuprocaini hydrochloridum, *see* Cloridrato de oxibuprocaína, 1123
Oxybutynini hydrochloridum, *see* Cloridrato de oxibutinina, 1129
Oxytetracyclini hydrochloridum, *see* Cloridrato de oxitetraciclina, 1137

Palmitato de ascorbila, 2381
Palmitato de cetila, *see* Ceras/gorduras, 633
Pancreatina, pulverizada, 2391
Pancreatis pulvis, *see* Pancreatina, pulverizada, 2391
Pantotenato de cálcio, 2395
Papaverina, cloridrato, *see* Cloridrato de papaverina, 1147
Papaverini hydrochloridum, *see* Cloridrato de papaverina, 1147
Paracetamol, 2403
Paracetamolum, *see* Paracetamol, 2403
Paraffina microcristallina, *see* Ceras/gorduras, 633
Paraffinum solidum, *see* Ceras/gorduras, 633
Parafina sólida, *see* Ceras/gorduras, 633
Parafina, microcristalina, *see* Ceras/gorduras, 633
Pectina, 2411
PEG 1500, *see* Macrogol 1500, 2051
PEG 4000, *see* Macrogol 4000, 2057
Phenazonum, *see* Fenazona, 1561
Pheniramini maleas, *see* Maleato de feniramina, 2083
Phenobarbitalum, *see* Fenobarbital, 1579
Phenylalaninum, *see* L-fenilalanina, 2023
Phenylbutazonum, *see* Fenilbutazona, 1567
Phenylephrini hydrochloridum, *see* Cloridrato de fenilefrina, 1013
Phenytoinum, *see* Fenitoína, 1573
Pilocarpina, cloridrato, *see* Cloridrato de pilocarpina, 1153
Pilocarpini hydrochloridum, *see* Cloridrato de pilocarpina, 1153
Piridoxal-5-fosfato, 2415
Piridoxina, cloridrato, *see* Cloridrato de piridoxina, 1159
Polietilenoglicol 1500, *see* Macrogol 1500, 2051
Polietilenoglicol 4000, *see* Macrogol 4000, 2057
Polimixina B, sulfato, *see* Sulfato de polimixina B, 2749
Poloxamera, *see* Poloxâmero, 2421

Poloxâmero, 2421
Polymyxini B sulfas, *see* Sulfato de polimixina B, 2749
Povidona, 2427
Povidonum, *see* Povidona, 2427
Povidonum iodinatum, *see* Iodopovidona, 1943
Prasterona, 2435
Prasteronum, *see* Prasterona, 2435
Praziquantel, 2443
Praziquantelum, *see* Praziquantel, 2443
Prednicarbato, 2447
Prednicarbatum, *see* Prednicarbato, 2447
Prednisolona, 2469
Prednisolona, acetato, *see* Acetato de prednisolona, 89
Prednisolona, hemisuccinato, *see* Hemissuccinato de prednisolona, 1821
Prednisoloni acetas, *see* Acetato de prednisolona, 89
Prednisoloni hydrogenosuccinas, *see* Hemissuccinato de prednisolona, 1821
Prednisoloni natrii phosphas, *see* Fosfato dissódico de prednisolona, 1621
Prednisolonum, *see* Prednisolona, 2469
Prednisona, 2489
Pregnenolona, 2495
Pregnenolonum, *see* Pregnenolona, 2495
Prilocaini hydrochloridum, *see* Cloridrato de prilocaína, 1165
Prilocaína, 2501
Prilocaína, cloridrato, *see* Cloridrato de prilocaína, 1165
Procaini hydrochloridum, *see* Cloridrato de procaína, 1171
Procaína, cloridrato, *see* Cloridrato de procaína, 1171
Progesterona, 2505
Progesteronum, *see* Progesterona, 2505
Prolina, 2525
Prolinum, *see* Prolina, 2525
Propifenazona, 2531
Propionato de clobetasol, 2537
Propionato de testosterona, 2561
Propranolol, cloridrato, *see* Cloridrato de propranolol, 1179
Propranololi hydrochloridum, *see* Cloridrato de propranolol, 1179
Propylis parahydroxybenzoas, *see* 4-hidroxibenzoato de propila, 33
Propyphenazonum, *see* Propifenazona, 2531
Proteinato de prata, 2573
Pyridoxini hydrochloridum, *see* Cloridrato de piridoxina, 1159
Quetiapina, fumarato, *see* Fumarato de quetiapina, 1649
Quetiapini fumaras, *see* Fumarato de quetiapina, 1649
Quinidina, sulfato di-hidratado, *see* Sulfato de quinidina di-hidratado, 2757
Quinina, cloridrato di-hidratado, *see* Cloridrato de quinina di-hidratado, 1191
Quinina, sulfato, *see* Sulfato de quinina, 2763
Quinolina amarela, 2579

Resorcinol, 2585
Resorcinolum, *see* Resorcinol, 2585
Riboflavina, 2593
Riboflavini natrii phosphas hydricum, *see* Fosfato sódico de riboflavina hidratado, 1629
Riboflavinum, *see* Riboflavina, 2593
Ropivacaini hydrochloridum monohydricum, *see* Cloridrato de ropivacaína monoidratado, 1197
Ropivacaína, cloridrato monoidratado, *see* Cloridrato de ropivacaína monoidratado, 1197

Sacarina sódica, 2601
Sacarose, 2609
Saccharinum natricum, *see* Sacarina sódica, 2601
Saccharum, *see* Sacarose, 2609
Salbutamol, sulfato, *see* Sulfato de salbutamol, 2769
Salbutamoli sulfas, *see* Sulfato de salbutamol, 2769
Salicilato de sódio, 2629
Scopolamini hydrobromidum, *see* Bromidrato de hioscina, 539
Selênio levedura, *see* Levedura de selênio, 2005
Serina, 2635
Serinum, *see* Serina, 2635
Sildenafila, citrato, *see* Citrato de sildenafila, 747
Sildenafili citras, *see* Citrato de sildenafila, 747
Solani amylum, *see* Amido, 351
Sorbato de potássio, 2641
Sorbitan stearate, *see* Monoestearatos, 2257
Sorbitani stearas, *see* Monoestearatos, 2257
Sorbitol, 2655
Sotalol, cloridrato, *see* Cloridrato de sotalol, 1201
Sotaloli hydrochloridum, *see* Cloridrato de sotalol, 1201
Span 60, *see* Monoestearatos, 2257
Sulfacetamida, 2663
Sulfacetamidum, *see* Sulfacetamida, 2663

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*

Sulfadiazina, 2669
Sulfadiazinum, *see* Sulfadiazina, 2669
Sulfato de anfetamina, 2675
Sulfato de atropina, 2683
Sulfato de colistina, 2689
Sulfato de condroitina sódico, 2695
Sulfato de dexanfetamina, 2699
Sulfato de gentamicina, 2705
Sulfato de glicosamina cloreto de potássio, 2723
Sulfato de glucosamina cloreto de potássio, *see* Sulfato de glicosamina cloreto de potássio, 2723
Sulfato de magnésio hepta-hidratado, 2727
Sulfato de manganês monoidratado, 2733
Sulfato de neomicina, 2737
Sulfato de polimixina B, 2749
Sulfato de quinidina di-hidratado, 2757
Sulfato de quinina, 2763
Sulfato de salbutamol, 2769
Sulfato de sódio deca-hidratado, 2773
Sulfato de tobramicina, 2779
Sulfato de zinco hepta-hidratado, 2785
Sulfoguaiacolato de potássio, 2791
Sulfoguaiacolum hydricum, *see* Sulfoguaiacolato de potássio, 2791
Sulpirida, 2797
Sulpiridum, *see* Sulpirida, 2797
SyrSpend® SF Alka, *see* Amido, 351
SyrSpend® SF pH4, *see* Amido, 351
SyrSpend® SF pH4 neo, *see* Amido, 351

Tacrolimo monoidratado, 2801
Tacrolimusum monohydricum, *see* Tacrolimo monoidratado, 2801
Tanino, 2807
Tanninum, *see* Tanino, 2807
Tartarato de L-Carnitina, 2817
Tartarato de L-carnitina, *see* Tartarato de L-Carnitina, 2817
Tartarato de Levocarnitina, *see* Tartarato de L-Carnitina, 2817
Tartarato de metoprolol, 2821
Taurina, 2827
Teofilina, 2833
Teofilina etilenodiamina hidratada, 2839
Testosterona, 2845
Testosterona, propionato, *see* Propionato de testosterona, 2561
Testosteroni propionas, *see* Propionato de testosterona, 2561
Testosteronum, *see* Testosterona, 2845
Tetraborato de sódio, 2853
Tetracaini hydrochloridum, *see* Cloridrato de tetracaína, 1205
Tetracainum, *see* Tetracaína, 2859
Tetracaína, 2859
Tetracaína, cloridrato, *see* Cloridrato de tetracaína, 1205
Tetraciclina, cloridrato, *see* Cloridrato de tetraciclina, 1221
Tetracyclini hydrochloridum, *see* Cloridrato de tetraciclina, 1221
Theobromatis oleum, *see* Ceras/gorduras, 633
Theophyllinum, *see* Teofilina, 2833
Theophyllinum et ethylendiaminum hydricum, *see* Teofilina etilenodiamina hidratada, 2839
Thiomersalum, *see* Timerosal, 2869
Threoninum, *see* L-treonina, 2045
Thymolum, *see* Timol, 2875
Tiamina, cloridrato de cloreto, *see* Cloridrato de cloreto de tiamina, 947
Timerosal, 2869
Timol, 2875
Tirosina, 2883
Tirotricina, 2889
Tobramicina, sulfato, *see* Sulfato de tobramicina, 2779
Tobramycini sulfas, *see* Sulfato de tobramicina, 2779
Tosilcloramida sódica, 2895
Tosylchloramidum natricum, *see* Tosilcloramida sódica, 2895
Treonina levógira, *see* L-treonina, 2045
Tretinoinum, *see* Tretinoína, 2901
Tretinoína, 2901
Triamcinoloni acetonidum, *see* Triancinolona acetonido, 2923
Triamcinolonum, *see* Triancinolona, 2917
Triancinolona, 2917
Triancinolona acetonido, 2923
Triclosan, 2953
Triclosanum, *see* Triclosan, 2953
Triptofano, 2983
Tritici amylum, *see* Amido, 351
Trometamina, *see* Trometamol, 2989
Trometamol, 2989
Trometamolum, *see* Trometamol, 2989
Tropicalamida, 3001
Tropicamidum, *see* Tropicalamida, 3001
Tyrosinum, *see* Tirosina, 2883
Tyrothricinum, *see* Tirotricina, 2889

Ubidecarenona, 3007
Ureia, 3013
Ureum, *see* Ureia, 3013
Ursodiol, *see* Ácido ursodeoxicólico, 285

Valerato de betametasona, 3041
Valerato de estradiol, 3071
Valina, 3081
Valinum, *see* Valina, 3081
Vancomicina, cloridrato, *see* Cloridrato de vancomicina, 1231

Vancomycini hydrochloridum, *see* Cloridrato de vancomicina, 1231
Vanilina, 3087
Vanillinum, *see* Vanilina, 3087
Vitamina C (ácido ascórbico), *see* Ácido ascórbico, 145
Vitamina E acetato pó 50%, *see* Concentrado seco de acetato de alfa-tocoferol, 1299

Xilitol, 3093
Xilometazolina, cloridrato, *see* Cloridrato de xilometazolina, 1237
Xilose, 3099
Xylitolum, *see* Xilitol, 3093
Xylometazolini hydrochloridum, *see* Cloridrato de xilometazolina, 1237
Xylosum, *see* Xilose, 3099

Zinci acetas dihydricus, *see* Acetato de zinco di-hidratado, 115
Zinci gluconas, *see* Gluconato de zinco, 1763
Zinci stearas, *see* Estearato de zinco, 1521
Zinci sulfas heptahydricus, *see* Sulfato de zinco hepta-hidratado, 2785
Zincum oroticum dihydricum, *see* Orotato de zinco di-hidratado, 2371

Ácido 4-aminobenzoico, 133
Ácido acetilsalicílico, 137
Ácido aminolevulínico, cloridrato, *see* Cloridrato do ácido 5-aminolevulínico, 1245
Ácido ascórbico, 145
Ácido aspártico, 153
Ácido benzoico, 157
Ácido bórico, 163
Ácido cítrico, 169
Ácido cítrico monoidratado, 193
Ácido esteárico 50, 201
Ácido fusídico, 213
Ácido fólico hidratado, 207
Ácido glutâmico, 219
Ácido nicotínico, 225
Ácido oxálico, 231
Ácido retinoico, *see* Tretinoína, 2901
Ácido salicílico, 237
Ácido sórbico, 261
Ácido tartárico, 269
Ácido tranexâmico, 279
Ácido ursodeoxicólico, 285
Ácido Ursodesoxicólico, *see* Ácido ursodeoxicólico, 285
Álcoois de cera de lã, 305
Álcool cetilestearílico, *see* Álcool cetoestearílico, 311
Álcool cetoestearílico, 311
Álcool cetoestearílico (tipo A), emuls, *see* Álcool cetoestearílico, 311
Álcool cetílico, *see* Álcool cetoestearílico, 311
Álcool emulsificante não iônico, 327
Éter gliceril guaiacol, *see* Guaifenesina, 1803

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *175-2.9-2025-01*